

Enhancing the Optical and Structural Properties of CdTe Thin Films via Thermal Treatments for Solar Cell Applications

DALAL N. ALHILFI ^{1*}, ALAA S. AL-KABBI ²

¹polymer Research Centre, University of Basrah, Basrah, Iraq,61004

²Department of Physics, College of Science, University of Basrah, Basrah, Iraq,61004

DOI: <https://doi.org/10.5281/zenodo.14546920>

Published Date: 23-December-2024

Abstract: This study examined the optical, structural, morphological, and electrical properties of polycrystalline cadmium telluride films fabricated using electrochemical deposition in a two-electrode system. Cadmium acetate is a source of cadmium and is one of the few precursors used to prepare cadmium tellurides. CdTe films were grown on glass substrates of fluorinated tin oxide (FTO), followed by thermal annealing at 200, 300, 350, and 400 °C. In addition, chlorination treatment was conducted at 400 °C. We analyzed various physical properties using characterization techniques, such as transmittance, X-ray diffraction, scanning electron microscopy with energy-dispersive X-ray spectroscopy (EDX), and a source meter. The increase in temperature after cadmium telluride deposition increased the optical transmittance, resulting in a progressive decrease in the optical energy bandgap from 1.74 to 1.49 eV. We computed various dielectric and optical constants using the Swanepoel and Herve-Vandamme models necessary for dielectric theory. Thermal annealing improved the crystallinity of the films (cubic structure), with 111 orientations being predominant. The heat treatment also determined and examined the various crystallinity parameters in detail. Surface morphology analysis revealed that the films exhibited homogeneity, high compaction, uniformity, and the absence of crystal imperfections.

Keywords: CdTe, optical bandgap, refractive index, photovoltaic, absorber layer, electrochemical deposition.

1. INTRODUCTION

The Shockley-Queisser limit can improve the conversion efficiency of cadmium-based thin-film solar cells while lowering the cost of traditional silicon solar cell technology. Cadmium telluride (CdTe), a member of the compound II-VI group, is increasingly popular in bulky photovoltaic technology because of its unique properties.[1] CdTe is a promising material because its bandgap is approximately 1.45 eV, which fits well with the solar spectrum. [2]. Other advantages of CdTe include its low cost, excellent stability, and simple deposition process. These qualities have enabled its application in thin-film solar cells, which are the advancements required to lower solar energy production costs.[3,4]

Various methods[5–8] in addition, Chemical Molecular Beam Deposition (CMBD) [9]Successive Ionic Layer Adsorption and Reaction (SILAR) [10,11], Chemical Bath Deposition (CBD) [12,13].and electrodeposition[14] Electrochemical deposition has emerged as a cost-effective and environmentally friendly method, making it ideal for the mass production of solar cells.[15]. Moreover, electrochemical deposition provides precise control over the film thickness and composition, which helps improve device performance.[16]. In this case (without a reference electrode), we employed a two-electrode electrochemical deposition method instead of a conventional three-electrode setup. Among other advantages, the two-electrode ED method can be used industrially in less time and with simpler systems. This increases efficiency and reduces metal ions from the reference electrode, lowering cost.[17,18]

Many studies have been conducted on cadmium telluride films using different types of cadmium, including cadmium chloride (CdCl₂) [19], cadmium nitrate Cd(NO₃)₂ [20], and cadmium sulfate (CdSO₄) [21,22]However, research on the use of cadmium acetate in cadmium telluride films is limited. Most investigations have focused on the effect of deposition agents on film properties.

Previous studies have shown that thermal annealing significantly improves CdTe thin films' crystallinity and optical properties.[23] Studies have shown that the annealing temperature induces grain size and defect density. [24] Performance in Solar Cell Applications. [25] This work builds on these findings by investigating the effects of thermal annealing at different temperatures on the structure and optical properties of CdTe films electrochemically deposited using cadmium acetate. The chemical and structural properties of the CdTe layer, such as thickness, deposition technique, substrate material, annealing process, substrate temperature, and CdCl₂ treatment, can have a significant impact. [26–28]

This study sought to understand the effect of annealing and chlorine treatment on the structural and optical properties of cadmium telluride (CdTe) films deposited using cadmium acetate (Cd(CH₃COO)₂). We will explore how different thermal treatments enhance film crystallinity, grain size, defect density, and optical performance. The goal was to gain deeper insights into the mechanisms by which thermal treatment enhances the properties of CdTe films, ultimately contributing to the activation of solar cells using these materials.

2. EXPERIMENTAL METHODS

2.1 Sample preparation

Thin films were prepared via electrochemical deposition in a two-electrode glass cell. The working electrode consisted of fluorinated tin oxide (FTO), and platinum (Pt) was used as the counter electrode. Both electrodes were ultrasonically cleaned for 20 min with acetone, ethyl alcohol, and deionized water before deposition. To prepare CdTe thin films, a 0.2 M cadmium source solution was prepared by dissolving 21 g of Cd(CH₃COO)₂ in 400 mL of deionized water. In parallel, 1.3 g of TeO₂ was dissolved in concentrated sulfuric acid (H₂SO₄) and then diluted with deionized water to create a 0.1 M TeO₂ solution. For deposition, 100 mL of Cd solution was combined with 1 mL of TeO₂ solution under constant stirring, and hydrochloric acid (HCl) was added dropwise until the pH reached two. The working and counter electrodes were positioned within 0.5 mm during deposition, and the films were grown at ambient temperature for 30 min under an applied voltage of -2 V ± 0.2 V. Characterization of Thin Films.

X-ray diffraction (XRD) analysis was performed using a 3064 XPERT-PRO diffractometer with Cu K α radiation to determine the structural properties of the films by analyzing the angles between 10° and 70°. The surface morphology was studied using field-emission scanning electron microscopy (FESEM) with JEOL JSM-6360A and ZEISS systems operating at 20 kV. Elemental Cd, Te, and Se analyses were conducted via energy-dispersive X-ray spectroscopy (EDS) using the same FESEM instruments.

Microstructural analysis was performed using A1-A6, a Raman spectrophotometer (Invia Renishaw) with a laser wavelength of 532 nm. The optical properties were measured using a JASCO V770 UV spectrophotometer, and the photoluminescence (PL) spectrum in the visible range was recorded using a computer-controlled LS-55 luminescence spectrophotometer (PerkinElmer Instruments)

2.2 Annealing processes

CdTe thin films were annealed at four different temperatures (200, 300, 350, and 400 °C) in an ambient environment using a temperature-controlled furnace with an additional CdCl₂ treatment at 400 °C. To simplify referencing the various models, each sample was assigned a specific code: A1 for the base sample, A2 for those heated at 200°C, A3 at 300°C, A4 at 350°C, and A6 for the CdCl₂ treatment at 400 °C. Figure 1 illustrates the setup preparation method, and Figure 2 depicts the CdCl₂ treatment process.

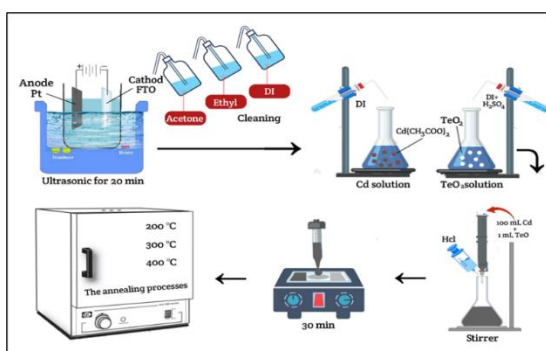


Figure 1: Steps of Preparation Methods

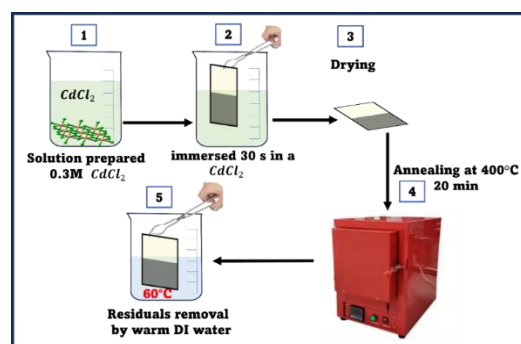


Figure 2: Schematic of CdCl₂ treatment

3. RESULTS AND DISCUSSION

3.1 XRD Analysis

Figure 3 Shows the XRD patterns of all the CdTe thin film samples (A1-A6). Each sample (A1-A6) showed five distinct diffraction peaks at $2\theta = 23.57^\circ, 39.16^\circ, 46.22^\circ, 62.22^\circ,$ and 71.11° , which corresponded to the (111), (220), (400), (331), and (422) planes of the cubic structure (JCPDS 15-0770 and JCPDS 75-2086). Sample A2 also exhibited peaks indicative of an orthorhombic phase at $2\theta = 34.2^\circ$ and 44.4° (JCPDS 41-0941). Moreover, hexagonal Te peaks were observed in samples A1-A5 at $2\theta = 45.39^\circ, 47.44^\circ,$ and 67.09° (JCPDS No. 894899), respectively, which diminished as the annealing temperature increased. These treatments enhance the crystalline quality and improve the films' electrical and optical properties.[29-31]. Notably, in sample A6, these hexagonal peaks vanished, and the intensity of the prominent peaks increased, along with new peaks at $2\theta = 35.54^\circ$, corresponding to ClO_2 . The enhancement of the crystal structure of the thin film following Cl treatment is likely due to interactions between chlorine and the grain boundaries, which aid in reducing or eliminating defects, thus enhancing performance and promoting recrystallization. [8,32].

The reaction between CdTe and oxygen resulted in peaks similar to those observed for CdTeO_3 , as noted in [33], and matched the positions listed on the cards (00-022-0129 and 00-020-1301) at 2θ angles of $20.86^\circ, 33.38^\circ, 49.47^\circ, 51.3^\circ,$ and 37.94° . As the annealing temperature increases, the crystal size also increases, enhancing the properties of the CdTe thin films as absorbent layers suitable for highly efficient CdTe-based solar cells. This increase in grain size helped reduce losses related to parasitic resistance. The sample intensities indicate high crystallinity with preferential growth in a specific orientation. The absence of contaminants in the materials produced suggested the presence of high-quality CdTe.[34,35]

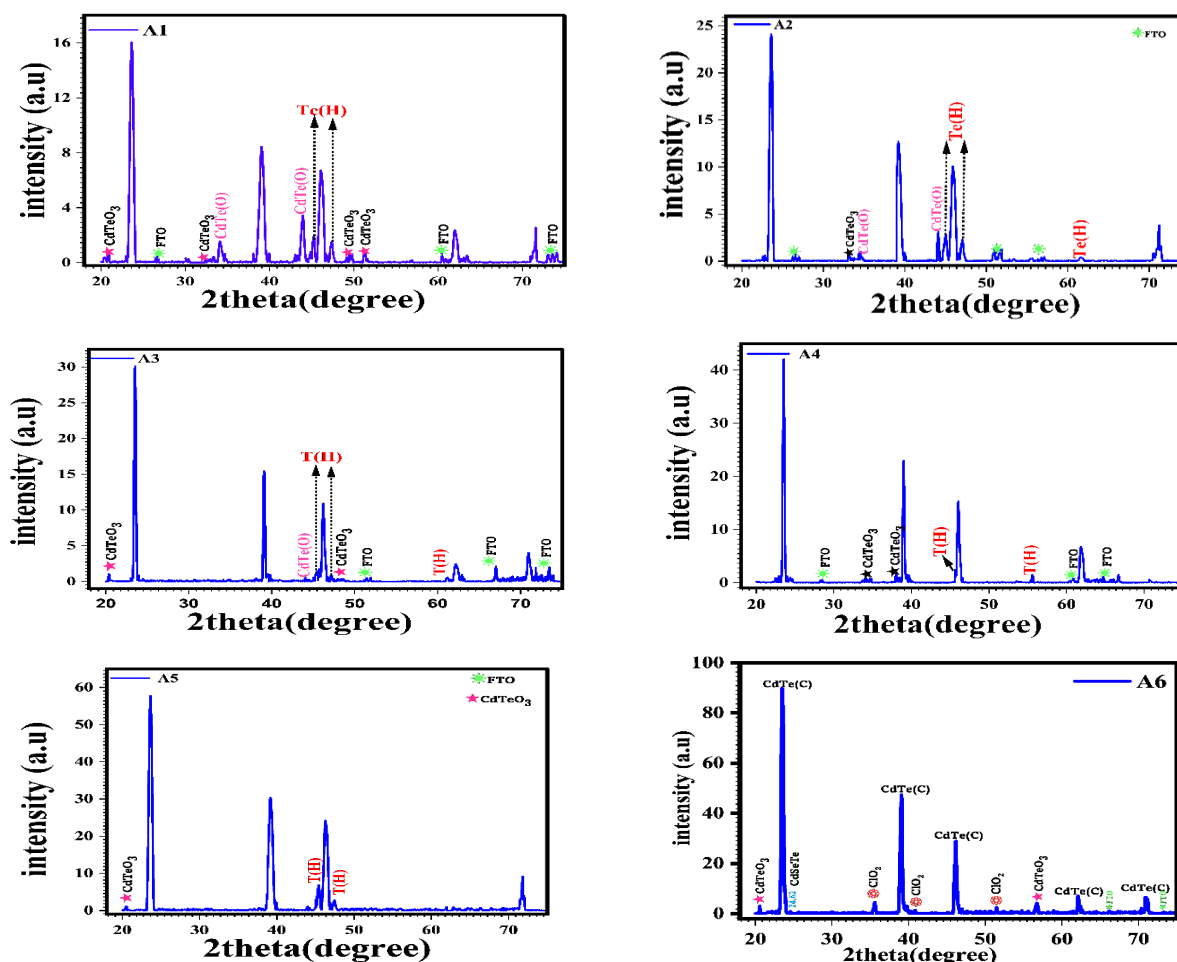


Figure 3: XRD pattern for CdTe thin film (A1-A6).

The average crystallite size (D) of the thin films was calculated using the Debye–Scherrer formula in Equations (1) [36].

$$D = \frac{0.9\lambda}{\beta \cos\theta} \tag{1}$$

Where λ is the wavelength of the Cu $K\alpha$ line, θ is the diffraction angle, and β is the full width at half maximum. The crystal sizes of the CdTe thin films were 19-41 nm. The ϵ values were calculated using Eq. (2).

$$\epsilon = \frac{\beta}{4\tan\theta} \tag{2}$$

The dislocation density (δ), which measures the number of defects in the thin films, was calculated from the crystallite size using Equation (3) [37].

$$\delta = \frac{1}{D^2} \tag{3}$$

Scherrer's formula indicates that D is the average size of a crystallite; the number of crystals per unit area was calculated via Equation (4):[38]

$$N = \frac{d}{D^3} \tag{4}$$

When the annealing temperature increased, the dislocation density decreased. This reduction indicates fewer crystal defects and a high-quality crystalline structure. At A1, δ is 29.7263×10^{13} lines.m⁻²; after chlorine treatment at 400°C, δ decreases to 2.30×10^{13} lines.m⁻², indicating a significant improvement. Conversely, the number of atoms per area (N) decreases with heat and chlorin treatment from 2.4×10^{16} m² to 0.21×10^{16} m², indicating a more tightly packed crystal lattice with fewer defects. These treatments increase the grain size, reduce the number of defects, and improve the electrical and optical properties of films[30,31]. See *Figure 4* *Figure 5* The lattice parameter (a-cubic) for thin films was estimated from the relation (3-5) [39]

$$a = d\sqrt{h^2 + k^2 + l^2} \tag{5}$$

The data in Table 1 show that

Table The d-spacing and lattice parameters (a-axis) are still far away, indicating the crystal stability during heat treatment. Studies have shown that electrodeposited CdTe films benefit significantly from post-deposition treatments such as thermal annealing and CdCl₂.

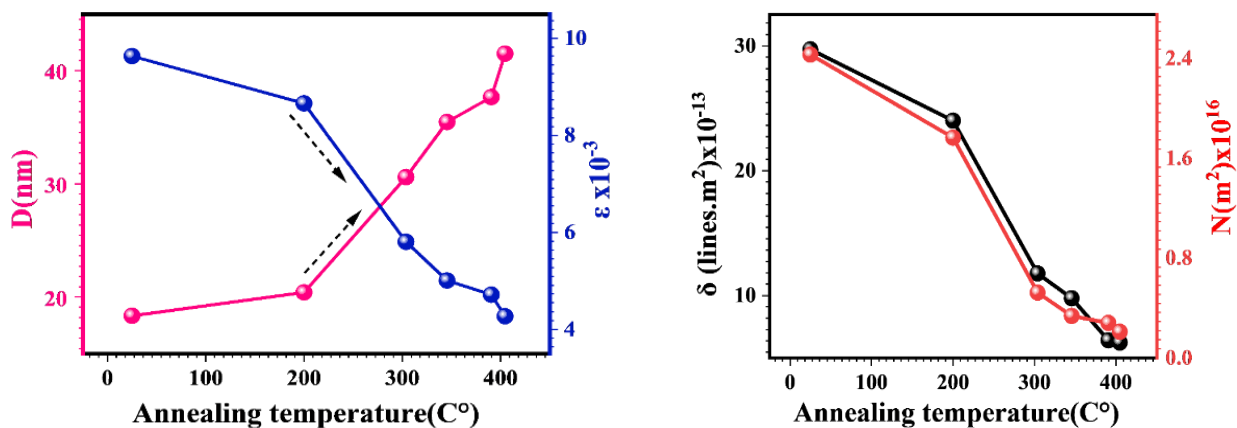


Figure 4: Grain size and microstrain with annealing temperature for A1-A6.

Figure 5: shows a change in dislocation and the number of atoms per area with an annealing temperature.

Table 1: XRD data for the CdTe thin films

Sam.	2θ (°)	β (°)	d [Å]	a [Å]	D nm	ε×10 ⁻³	δ×10 ⁻¹³ lines/m ²	N×10 ¹⁶ m ²
A1	23.65	0.46	3.74	6.48	18.34	9.63	29.72	2.43
A2	23.65	0.41	3.74	6.48	20.41	8.64	29.75	2.43
A3	23.53	0.27	3.75	6.5	30.59	5.8	10.7	0.52
A4	23.53	0.25	3.75	6.5	34.31	5.38	8.63	0.38
A5	23.53	0.23	3.74	6.48	37.67	4.71	8.63	0.38
A6	23.57	0.2	3.74	6.48	41.5	4.27	5.81	0.21

3.2 FESEM and EDX of CdTe thin films

Figure 6 FESEM images of CdTe thin films at different magnifications (200 and 500 nm) and their corresponding histograms show the statistical distribution of particle sizes across the film surfaces. For sample A1, the as-deposited film contained tangled nanowires with a particle size distribution around 21.14 nm, suggesting some variation in the size. After annealing at 200°C (A2), the particles transformed into rod-like structures with sizes ranging from 48.34 nm to 200 nm, and the distribution was more uniform, with an average size of 30.4 nm. The A3 film shows a mix of tiny nanorods (39.51 nm to 250 nm) with a mean size of 110.9 nm, indicating diverse lengths owing to the annealing conditions. Sample A4 exhibited a rough surface with a mixture of rods and particles; the average particle size was 115.1 nm, with rods averaging 367.91 nm in length. Annealing at 400°C (A5) enhances the granule structure, making the grains more spherical and distinct. The average particle size (116.34 nm) reflects improved crystallinity. After chloride treatment (A6), hexagonal structures with 40–60 nm diameters formed compacted grains with a mean particle size of 126.7 nm. The chloride treatment passivated the grain boundaries and improved the grain size and structural structure. These FESEM results align with the XRD findings, confirming that annealing and chloride treatment contribute to grain growth and enhanced structural properties.

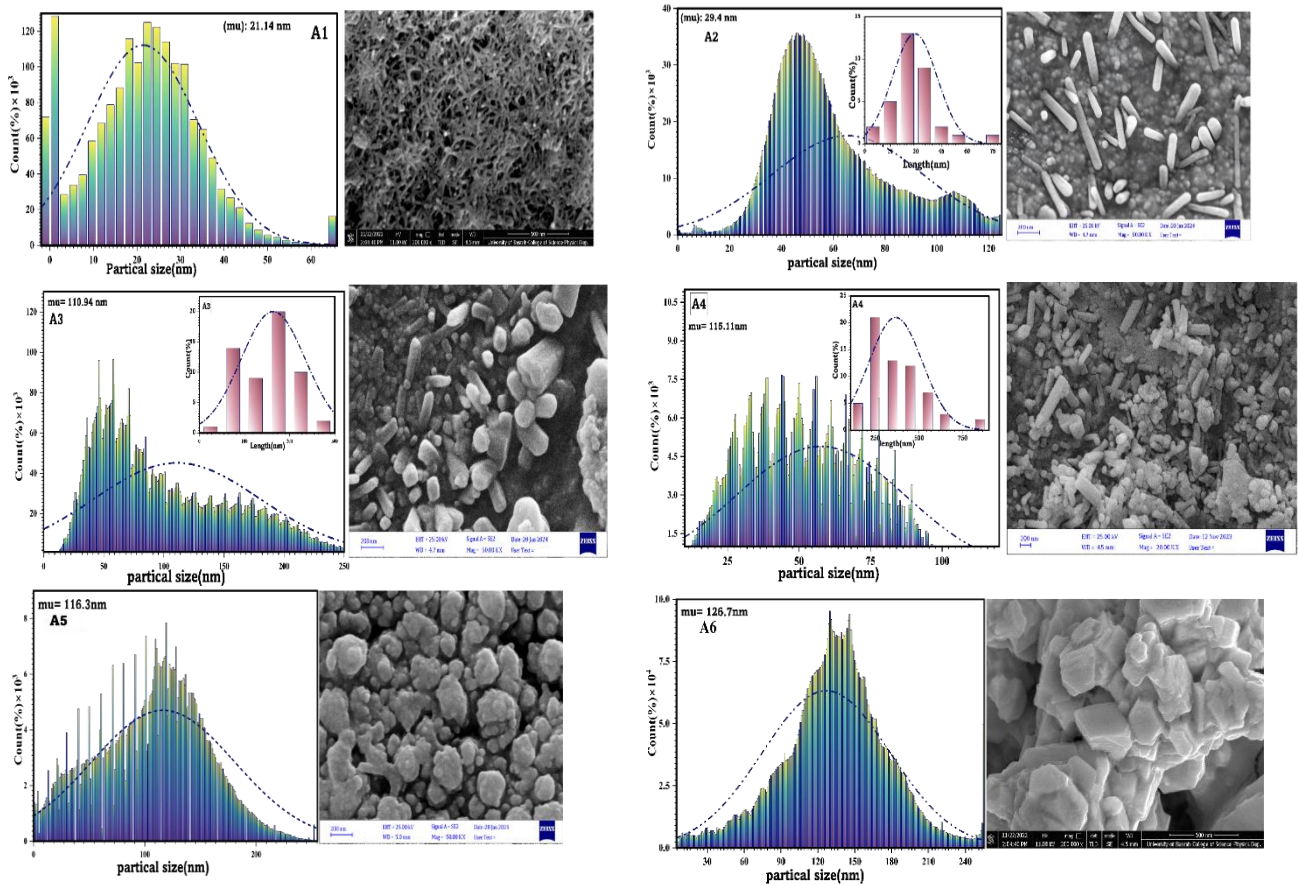


Figure 6: Histogram and FEMES image of CdTe thin films.

Quantitative analysis of the CdTe thin films was conducted using energy-dispersive X-ray spectroscopy (EDX) (Figure 7) **Figure 7**, which revealed the atomic compositions of the samples A1–A6. Sample A1, as-deposited, showed a higher atomic percentage of Te than Cd. The Cd ratio increases upon annealing, whereas the Te content decreases, particularly at higher annealing temperatures. For the chloride-treated sample at 400°C, the composition became nearly stoichiometric, likely owing to the volatilization of Te at this temperature (*Table*).

Table 2: Atomic ratios of CdTe thin films (A1-A6).

Sample	Te%	Cd%
A1	87.70	12.30
A2	75.50	24.50
A3	69.00	31.00
A4	65.10	34.90
A5	61.70	38.30
A6	53.50	46.60

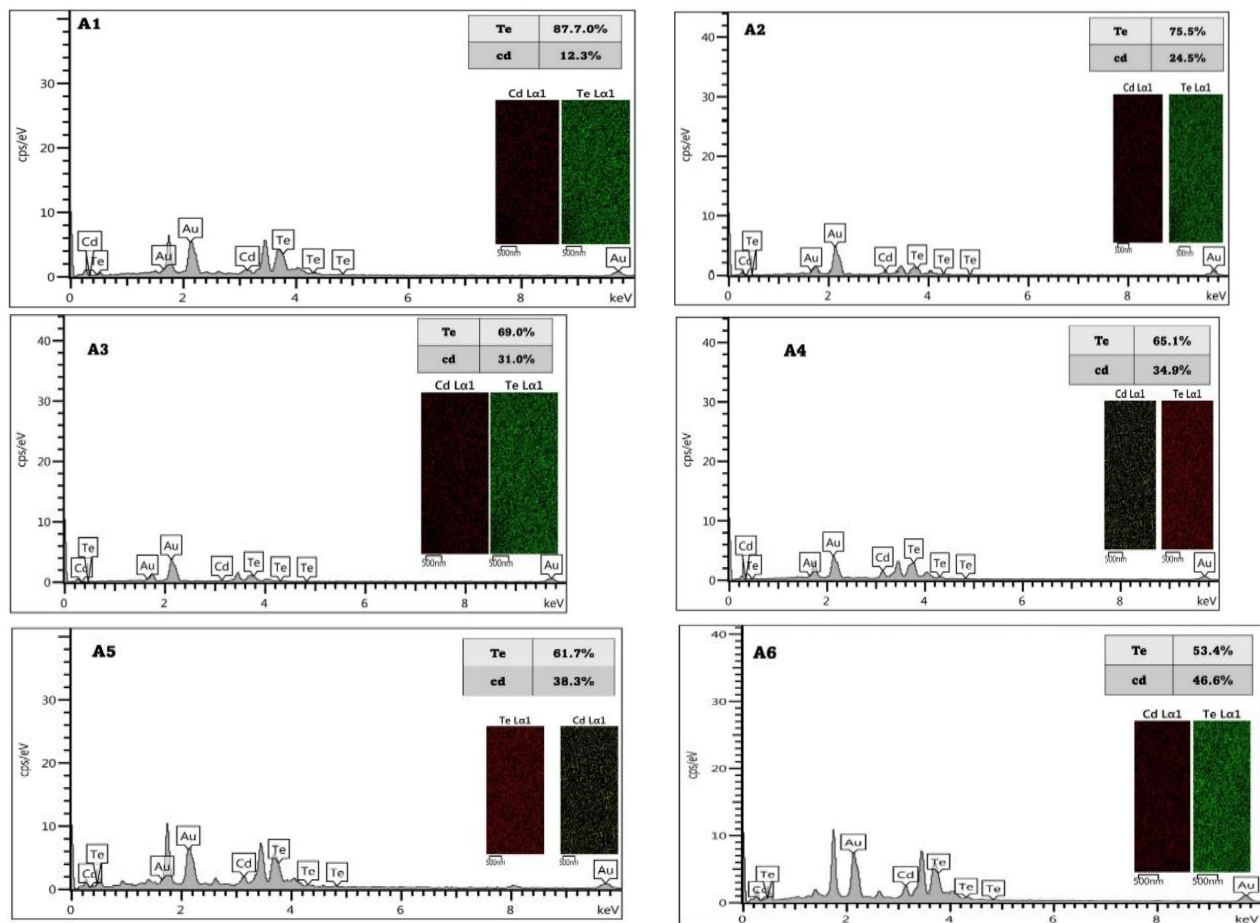


Figure 7: EDX analysis for CdTe samples (A1-A6)

3.3 Optical properties

3.3.1 Transmittance and Absorption Coefficient

Figure 8 illustrates the films' transmittance in the 400–900 nm range, revealing a steady profile in the low-wavelength region. An interference pattern emerges at higher wavelengths, suggesting that the film surfaces are uniform and smooth. Additionally, increasing the annealing temperature enhances the optical properties of the CdTe films, boosting their efficiency in optical and electronic applications. The absorption coefficient (α) was determined using Equation (6).[40]

$$\alpha = \frac{1}{d} \ln\left(\frac{1}{T}\right)$$

6

The absorption coefficients for samples A1-A6 demonstrate that α increases with increasing annealing temperature, suggesting that the thin film becomes more efficient at absorbing light. This is particularly evident in the absorption coefficient (α), which measures how effectively a material absorbs photons at a specific wavelength. With an increase in annealing temperature, the crystal structure of the CdTe thin film improved, enhancing its optical properties.

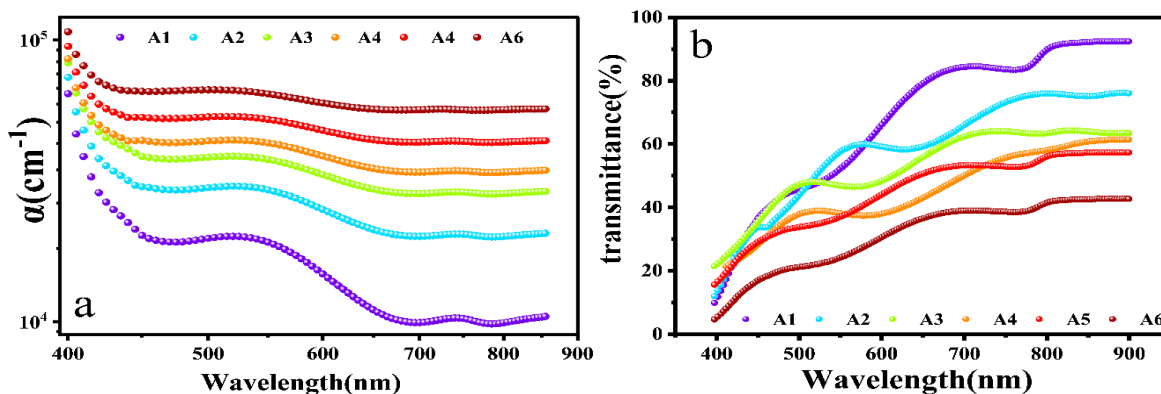


Figure 8: The absorption coefficient and transmittance spectra of CdTe thin films.

3.3.2 Optical Band Gap and Reflective Index

The optical band gap shown in Figure 9; for the CdTe electroploration, thin films (A1-A6) were obtained from the plot graph of $(\alpha h\nu)^2 \cdot h\nu$. [15]

$$(\alpha h\nu)^{1/n} = B[h\nu - E_g] \tag{7}$$

7

'B' remains constant for a specific material, while 'n' varies based on the type of electronic transition occurring. In this instance, the linear portion of the curve was extrapolated to intersect the axis at $(\alpha h\nu)^2 = 0$, representing the energy gap value associated with the direct transition, as indicated in Table This shift might be attributed to the annealing process, which improves the material's electronic properties by removing impurities and pinholes from the thin films and promoting recrystallization. [19,41].

The band gaps decreased following the heat and chlorine treatments. This reduction in E_g can be attributed to the annealing process, which enhances the material's electronic properties by eliminating impurities and pinholes from the thin films, achieving better stoichiometry, and increasing the grain size and orientation alignment, thereby improving the crystallinity of the thin film. After chlorine treatment and annealing at 400°C, the band gap value of the A6 thin film approaches 1.49 eV, which is within the theoretical range for CdTe thin films used as absorbers in solar cells.

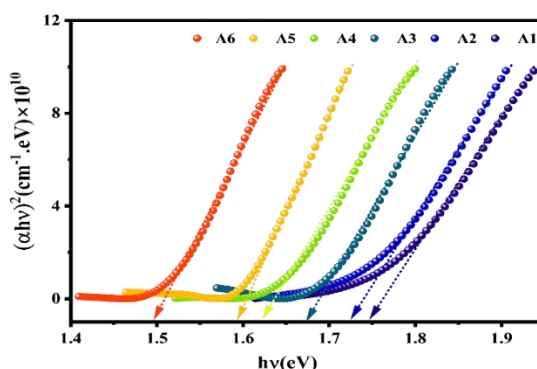


Figure 9: Optical band gap of CdTe thin films

The refractive index is an essential optical property that influences the permeability of thin films. This study employed two techniques to measure the refractive index of the thermally treated CdTe thin films: the Harve-Vandamme model.[42,43], and the Swanepoel method[44]The Harve-Vandamme model links the photo energy gap to the refractive index, illustrating how the energy gap affects optical properties. Conversely, the Swanepoel method determines the refractive index by eliminating interference patterns using transmittance spectra. Utilizing both methods provides mutual verification and ensures higher accuracy. This dual-method approach underscores the advantages of heat treatment, which enhances the

crystalline quality of CdTe films, thereby improving their optical and structural properties.[43,45]

The Herve–Vandamme model relates the reflective index (n) with the energy gap of materials and is mathematically given by the following equation.[46]:

$$n^2 = 1 + \left(\frac{A}{B + E_g} \right)^2$$

Error! No text of specified style in document.-8

The A and B constants are 13.6 eV and 3.4 eV, respectively.

Figure 10 Variation in Eg and refractive index for CdTe thin films annealing temperature (A1-A6) annealing temperature dependency See Table

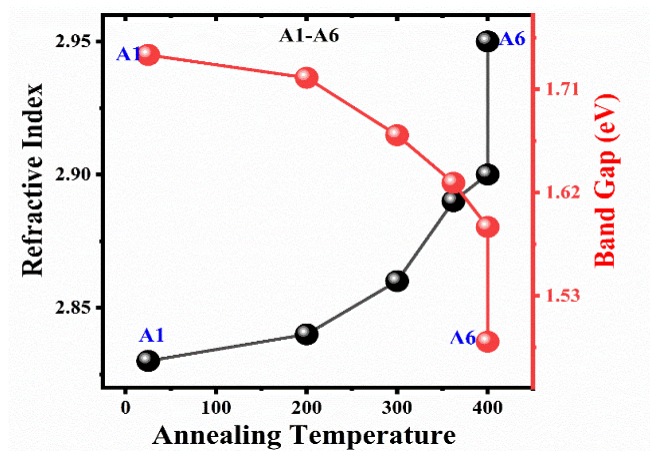


Figure 10: The Reflective Index for CdTe thin films (A1-A6) and bandgap vis annealing temperature.

Table 3: Optical energy band gap, refractive index, absorption coefficient, and extinction coefficient

Sample	Eg	n	α	ρ
	ev		cm ⁻¹	
A1	1.74	2.83	9.97×10 ⁴	1.02
A2	1.72	2.84	2.02×10 ⁵	1.023
A3	1.67	2.86	2.88×10 ⁵	1.027
A4	1.62	2.89	3.40×10 ⁵	1.032
A5	1.59	2.90	4.31×10 ⁵	1.034
A6	1.49	2.95	5.66×10 ⁵	1.04

The envelope method, developed by Swanepoel et al. [47,48], Equation (10) determines the refractive index (n). The Swanepoel method nullifies the interference pattern in the transmittance spectra via the envelope of the spectra and interference-free transmittance.[44,49]

$$n = \sqrt{N + (N^2 - S^2)^{1/2}} \tag{9}$$

$$\text{where } N = 2S \frac{T_M - T_m}{T_M T_m} + \frac{S^2 + 1}{2} \tag{10}$$

To calculate n in the weak and medium absorption regions, T_M and T_m values at different d values must be obtained. The transmission values should be read on the curves of T_M and T_m at each wavelength, not on the actual spectrum. The refractive index can be determined by measuring the transmission spectrum of the clean substrate alone and using the A1-A6 Equation (12) to calculate S.

$$s = \frac{1}{T_S} + \left(\frac{1}{T_S} - 1\right)$$

11

Where T is interference-free transmittance.

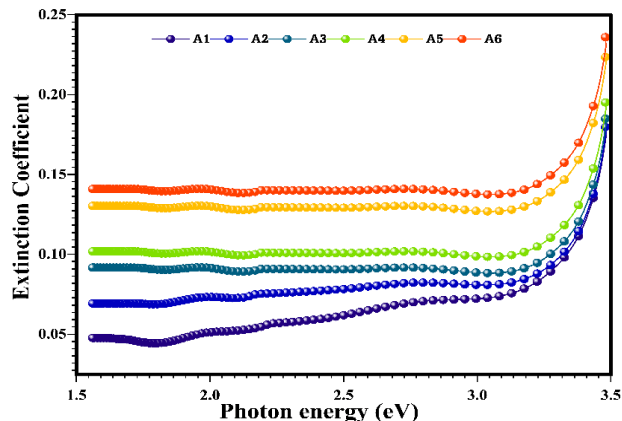
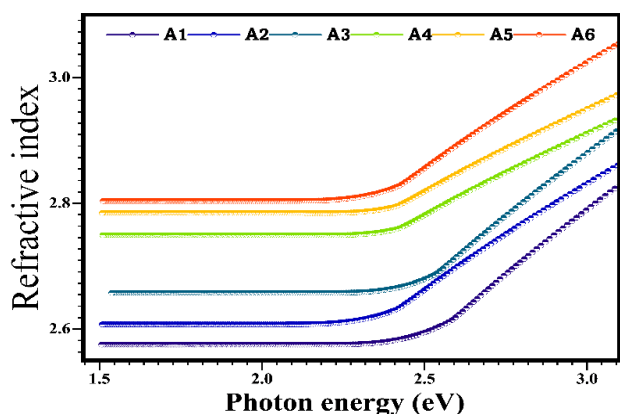


Figure 10: The refractive Indices of (A1-A6) vis photon energy. **Figure 11: The extinction coefficient vis photon energy of the CdTe (A1-A6)**

Refractive index data were obtained from the Swanepoel and Herve-Vandamme models. Both models show that the heat treatment increases the refractive index and lowers the optical energy gap. This implies that the film formed better, the crystals were more uniform, and the structure was more stable. The Swanepoel model shows that the refractive index varies with the wavelength, typically decreasing as the wavelength increases, depending on the annealing conditions. It reaches its peak values between 2.74 and 2.92, attributed to optical interference effects in the thin films and reduced material opacity at longer wavelengths. Conversely, the Herve-Vandamme model emphasizes the relationship between a material's electronic structure and refractive index. According to this model, increasing the annealing temperature enhances crystallinity and reduces structural defects, predicting refractive index values between 2.83 and 2.95, mainly when treated with CdCl₂ at 400°C. This indicates a strong link between improved structural properties and higher optical density.[47,50]

The Swanepoel and Harvey-Vandamme models exhibit a similar pattern in refractive index changes, albeit through different approaches. Swanepoel concentrates on optical interference and spectral characteristics, whereas Harvey-Vandamme prioritizes the electron structure. Together, these models provide a thorough understanding of the optical properties of CdTe thin films, underscoring the significance of thermal treatments in improving their performance in optoelectronic devices like solar cells and photodetectors...[44,49–51]

In a 2016 study, it was discovered that heating CdTe films to 150, 250, and 350 °C enhanced their optical transmittance. The optical energy gap was reduced from 1.78 eV to 1.54 eV, and the refractive index increased from 2.77 to 2.89. These changes were attributed to improved crystallinity and grain growth, making the films more suitable for optoelectronic applications.[52]

Table 4 This paper compares the refractive indices, preparation methods, and sources of Cd and Te across studies. It shows that CdTe films fabricated by electrodeposition with CdCl₂ treatment work better than others because they have better optical bandgaps and refractive index values. This makes them better suited for use in solar-energy applications. The CdCl₂ treatment notably improves the films' optical and structural properties, enhancing their suitability for photovoltaic applications.[53,54]

Table 4: Compares each study regarding the preparation techniques employed, sources of CdTe, and refractive index.

Method	CdTe Source	(n)	Ref.
Thermal evaporation at high vacuum	CdTe powder	2.04-2.47	[54]

Thermal vacuum evaporation	CdTe powder	2.1-2.45	[55]
Electron beam evaporation	CdTe powder	2.46-2.52	[45]
Thermal vacuum evaporation	CdTe powder	2.77-2.89	[50]
Thermal vacuum evaporation	CdTe powder	2.86- .92	[56]
Electrodeposition	C4H6CdO4+TeO2	2.83 - 2.96	This study

The extinction coefficient (K) describes the amount of light absorbed or scattered as it passes through the material and is calculated. [57].

$$K = \frac{\alpha\lambda}{4\pi} = \frac{\lambda}{4\pi d} \ln(1/A) \tag{12}$$

Where α is the absorption coefficient, d is the film thickness, and A is the absorbance. The K value increased with an increase in the photon energy, and the annealing temperature in **Error! Reference source not found.** Follows the same trend. The extinction coefficient agrees well with [58].

3.3.3 Dielectric constant and Relative density

Figure 12 The dielectric constant is sensitive to the electronic structure of a material. This is directly related to the density of the state within the forbidden gap and the electromagnetic radiation that passes through it. Both the real (ϵ') and imaginary (ϵ'') components of the complex dielectric constant ($\epsilon = \epsilon' + i\epsilon''$) are intrinsic features of a material. The equation below shows that the dielectric constant can be calculated from the reflective index and the extinction coefficient. [59]

$$\epsilon' = n^2 - K^2 \tag{13}$$

$$\epsilon'' = 2K^2 \tag{14}$$

The real part of the dielectric constant reflects a material's ability to slow light, while the imaginary part represents energy absorption via dipole motion.[59]. Both parts of the dielectric constant increased as the photon energy and temperature increased. This is because CdTe thin films become more crystalline. The fundamental part is notably higher than the imaginary part, indicating the material's strong response to incident light.[53,55]

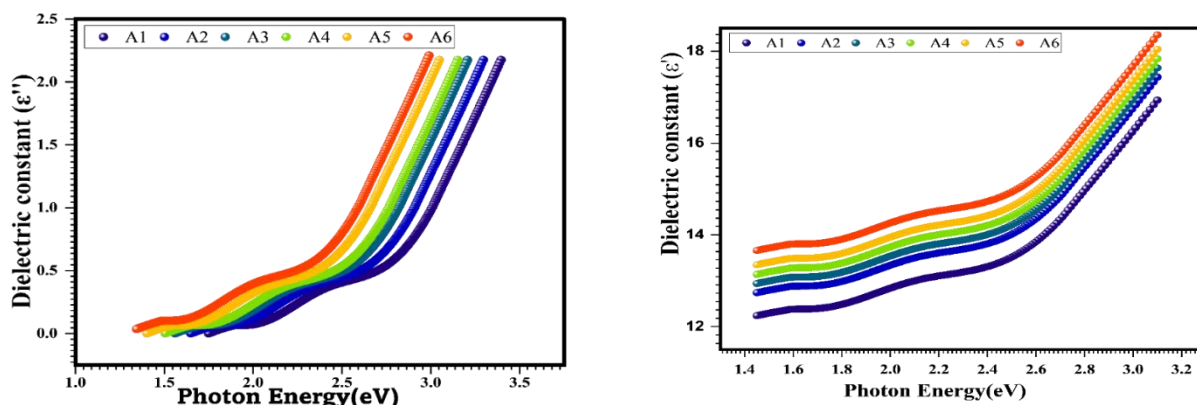


Figure 12: The real and imaginary parts of the dielectric for CdTe thin films according to the Swanepoel method.

The Lorentz–Lorentz formula was used to calculate CdTe thin films' relative density (ρ). [60].

$$\rho = \left(\frac{n_f^2-1}{n_b^2-1}\right) \left(\frac{n_b^2+1}{n_f^2+1}\right) \tag{15}$$

' n_b ' is the refractive index of bulk CdTe, 2.72, and ' n_f ' is the refractive index of deposited CdTe thin films.

Figure 13 Shows the CdTe thin films at various annealing temperatures and CdCl₂ treatments, with calculated relative densities ranging from 1.02 to 1.04(see Table 4). Annealing improved the film structure and slightly increased the relative density compared to the as-deposited state. At 400°C with CdCl₂ treatment, the films became more crystalline, reducing the defects and increasing the relative density to 1.04. These improvements in microstructure enhance the optical and electronic

properties, making the films suitable for applications like solar cells.[45,61].

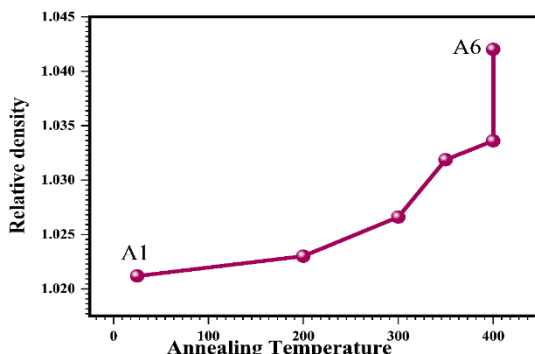


Figure 13: Variation in relative density with annealing temperature of CdTe thin films.

3.3.4 Energy loss functions

Dielectric theory outlines the surface energy loss function (SELF) and volume energy loss function (VELF). During inelastic scattering, these functions transfer energy to or from the outermost atomic layers of compound semiconductors. This process is driven by the excitation of electrons at the surface and interface. Both energy loss functions are assessed using the subsequent relations: Equations (17) and (18) are as follows: [52]

$$VELF = \frac{\epsilon''}{\epsilon'^2 + \epsilon''^2} \tag{16}$$

$$SELF = \frac{\epsilon''}{(\epsilon' + 1)^2 + \epsilon''^2} \tag{17}$$

The CdTe results show significant differences between the untreated and thermally treated samples, as shown in Figure 14. The untreated sample (A1) had a disordered surface, leading to high energy loss in the SELF plot. In contrast, the thermally treated samples exhibited lower self-energies and improved internal structures, which enhanced energy transport. The untreated sample also had the lowest VELF values owing to material defects, while the heat-treated samples showed higher VELF values, indicating better crystal quality. As the treatment temperature increased, the SELF values decreased, and the VELF values increased with increasing wavelength (700–800 nm). The improvements observed near the absorption edge matched the XRD results. This means that the heat treatment increased the number of grains and eliminated flaws, which improved the surface and bulk properties. [62–64]

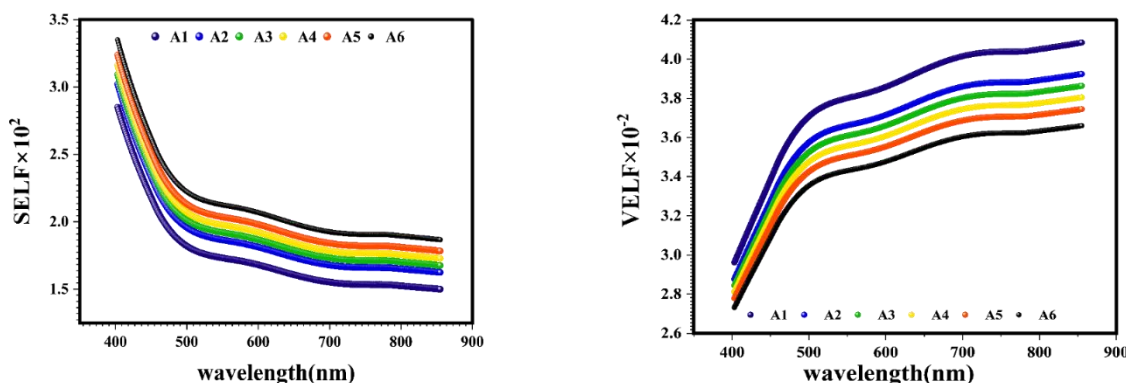


Figure 14: The energy loss function of CdTe thin films a SELF and b VELF

3.4 Photoluminescence spectroscopy

As shown in Figure 15, the CdTe thin films (A1–A6) emit light when excited at a wavelength of 503 nm. The band-edge

emission from flaws and incomplete crystallization caused a weak peak at approximately 680 nm in the (A1) thin film. After annealing at 200, 300, and 400°C and CdCl₂ for A6, the peak shifted to longer wavelengths as the annealing temperature increased. The binding energy of excitons increased as the size of the nanoparticles increased, as confirmed by other studies. [7,65,66] The full width at half maximum (FWHM), which is between 6.5 and 19.3 nm, increases after heating, which means that the material properties improve and the radiation transitions work better. The FWHM, which does not exceed 60 nm, further supports the high quality of the CdTe films. [67,68]

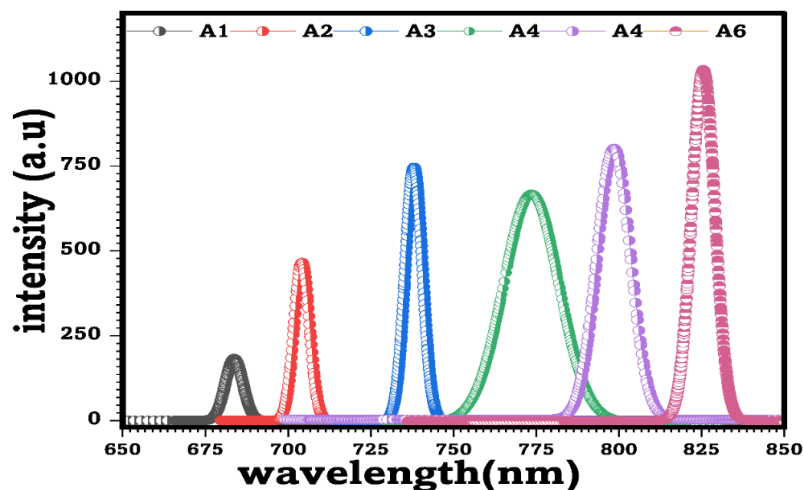


Figure 15: Emission spectra of the wavelength of CdTe (A1-A4).

4. CONCLUSION

This study seeks to understand the effects of increasing temperature on electrochemically deposited cadmium telluride thin films. The XRD patterns indicate that the cadmium telluride films retained their cubic lattice structure at different deposition temperatures. Higher annealing and chlorination temperatures, particularly 400 °C, led to larger grain sizes and fewer defects. The SEM images revealed that the temperature substantially impacted the surface morphology, with distinct differences observed at each treatment temperature.

At 400 °C, the optical bandgap decreased from 1.74 eV in the untreated A1 sample to approximately 1.49 eV in the chlorinated sample, indicating its enhanced suitability for solar cell applications. Owing to their improved crystallinity and light-absorption capabilities, these films are expected to be effective for high-efficiency photovoltaic devices.

We assessed the optical properties using both the Herve-Vandamme and Swanepoel methods. Electrochemical deposition using cadmium acetate and TeO₂ in these films results in a higher refractive index than other cadmium sources, necessitating higher annealing and chlorination temperatures. The Vandamme method provided more profound insights into the electronic properties of the films by exploring the relationship between the energy band gap and the refractive index. In contrast, the Swanepoel method analyzes the refractive index through transmittance spectra, which are significantly affected by surface features such as smoothness and uniformity, making it challenging to discern the film's internal structure. The findings of this study illustrate that electrochemical deposition coupled with thermal treatment and chlorination at 400 °C significantly improves the structural and electronic properties of CdTe thin films, outperforming previously reported deposition techniques. These results confirm the value of this approach in the fabrication of high-efficiency solar cells.

REFERENCES

- [1] Bibin John, S. Varadharajaperumal, Comprehensive Review on CdTe Crystals: Growth, Properties, and Photovoltaic Application, *Phys. Met. Metallogr.* 124 (2023) 1795–1812. <https://doi.org/10.1134/S0031918X2110094X>.
- [2] L. Verma, A. Khare, Photovoltaic applications of electrodeposited CdTe films: impact of deposition time, *Emergent Mater.* 7 (2024) 2065–2078. <https://doi.org/10.1007/s42247-024-00676-3>.
- [3] D. Suthar, S. Chuhadiya, R. Sharma, Himanshu, M.S. Dhaka, An overview on the role of ZnTe as an efficient interface in CdTe thin film solar cells: a review, *Mater. Adv.* 3 (2022) 8081–8107. <https://doi.org/10.1039/D2MA00817C>.

- [4] J. Wang, M. Isshiki, II–IV Semiconductors for Optoelectronics: CdS, CdSe, CdTe, in Springer Handb. Electron. Photonic Mater., Springer US, Boston, MA, 2006: pp. 829–842. https://doi.org/10.1007/978-0-387-29185-7_34.
- [5] F.P.N. Inbanathan, P. Kumar, K. Dasari, R.S. Katiyar, J. Chen, W.M. Jadwisieniczak, Ellipsometry study of CdSe thin films deposited by PLD on ito coated glass substrates, Materials (Basel). 14 (2021). <https://doi.org/10.3390/ma14123307>.
- [6] C. Doroody, K.S. Rahman, H.N. Rosly, M.N. Harif, K. Sopian, S.F. Abdullah, N. Amin, A comprehensive comparative study of CdTe thin films grown on ultra-thin glass substrates by close-spaced sublimation and RF magnetron sputtering, Mater. Lett. 293 (2021). <https://doi.org/10.1016/j.matlet.2021.129655>.
- [7] S.A. Fadaam, M.H. Mustafa, A.H. Abd AlRazaK, A.A. Shihab, Enhanced efficiency of CdTe Photovoltaic by thermal evaporation Vacuum, Energy Procedia 157 (2019) 635–643. <https://doi.org/10.1016/j.egypro.2018.11.229>.
- [8] A. Abbas, G.D. West, J.W. Bowers, P. Isherwood, P.M. Kaminski, B. Maniscalco, P. Rowley, J.M. Walls, K. Barricklow, W.S. Sampath, K.L. Barth, The effect of cadmium chloride treatment on close spaced sublimated cadmium telluride thin film solar cells, in: 2012 IEEE 38th Photovolt. Spec. Conf. PART 2, 2012 IEEE 38th Photovoltaic Specialists Conference (PVSC) PART 2, 2012: pp. 1–6. <https://doi.org/10.1109/PVSC-Vol2.2012.6656778>.
- [9] T.M. Razykov, K.M. Kuchkarov, C.S. Ferekides, B.A. Ergashev, R.T. Yuldoshov, N. Mamarasulov, M.A. Zufarov, Characterization of CdTe thin films with different compositions obtained by CMBD for thin film solar cells, Sol. Energy 144 (2017) 411–416. <https://doi.org/10.1016/j.solener.2017.01.047>.
- [10] S. Samanta, D.B. Salunke, S.R. Gosavi, R.S. Patil, Structural and Optoelectronic Properties of Nanocrystalline CdTe Thin Films Synthesized by Using SILAR Technique, J. Nano- Electron. Phys. 9 (2017) 05028-1-05028-4. [https://doi.org/10.21272/jnep.9\(5\).05028](https://doi.org/10.21272/jnep.9(5).05028).
- [11] Y. Suchikova, S. Kovachov, I. Bohdanov, E. Popova, A. Moskina, A. Popov, Characterization of CdxTeyOz/CdS/ZnO Heterostructures Synthesized by the SILAR Method, Coatings 13 (2023) 639. <https://doi.org/10.3390/coatings13030639>.
- [12] S. Surabhi, KumarAnurag, S. Rajpal, S.. Kumar, A new route for preparing CdTe thin films by chemical bath deposition, Mater. Today Proc. 44 (2021) 1463–1467. <https://doi.org/10.1016/j.matpr.2020.11.635>.
- [13] Z.S. Kachhia, S.H. Chaki, S.R. Patel, J.P. Tailor, Z.R. Parekh, M.P. Deshpande, Chemical bath deposited CdTe thin film: Optical, electrical, and photoresponse aspects, Next Mater. 3 (2024) 100152. <https://doi.org/10.1016/j.nxmate.2024.100152>.
- [14] S.S. Oluyamo, A.A. Faremi, O.I.O. Olusola, Y.A. Odusote, Tunability of conductivity type and energy band gap of CdTe thin film in the electrodeposition technique, Mater. Today Proc. 38 (2021) 558–563. <https://doi.org/10.1016/j.matpr.2020.02.962>.
- [15] D.N. Alhilfi, A.S. Al-Kabbib, Characterization and application of electrochemical deposition Cdse thin films, Chalcogenide Lett. 21 (2024) 641–649. <https://doi.org/10.15251/CL.2024.218.641>.
- [16] R. Sharma, Himanshu, S.L. Patel, M.D. Kannan, M.S. Dhaka, Effect of different annealing conditions on CdZnTe thin films for absorber layer applications, Surfaces and Interfaces 33 (2022) 102204. <https://doi.org/10.1016/j.surfin.2022.102204>.
- [17] R. Raccichini, M. Amores, G. Hinds, Critical review of the use of reference electrodes in li-ion batteries: A diagnostic perspective, Batteries 5 (2019). <https://doi.org/10.3390/batteries5010012>.
- [18] S. Saha, M. Johnson, F. Altayaran, Y. Wang, D. Wang, Q. Zhang, Electrodeposition Fabrication of Chalcogenide Thin Films for Photovoltaic Applications, Electrochem 1 (2020) 286–321. <https://doi.org/10.3390/electrochem1030019>.
- [19] H.I. Salim, V. Patel, A. Abbas, J.M. Walls, I.M. Dharmadasa, Electrodeposition of CdTe thin films using nitrate precursor for applications in solar cells, J. Mater. Sci. Mater. Electron. 26 (2015) 3119–3128. <https://doi.org/10.1007/>

s10854-015-2805-x.

- [20] T. Nishio, M. Takahashi, S. Wada, T. Miyauchi, K. Wakita, H. Goto, S. Sato, O. Sakurada, Preparation and characterization of electrodeposited in-doped CdTe semiconductor films, *Electr. Eng. Japan* 164 (2008) 12–18. <https://doi.org/10.1002/ej.20673>.
- [21] I. Dharmadasa, M. Madugu, O. Olusola, O. Echendu, F. Fauzi, D. Diso, A. Weerasinghe, T. Druffel, R. Dharmadasa, B. Lavery, J. Jasinski, T. Krentsel, G. Sumanasekera, Electroplating of CdTe Thin Films from Cadmium Sulphate Precursor and Comparison of Layers Grown by 3-Electrode and 2-Electrode Systems, *Coatings* 7 (2017) 17. <https://doi.org/10.3390/coatings7020017>.
- [22] L. Verma, A. Khare, Synthesis and characterization of CdTe thin film on FTO by electrodeposition technique for CdTe/CdS solar cells, *IOP Conf. Ser. Mater. Sci. Eng.* 798 (2020) 012021. <https://doi.org/10.1088/1757-899X/798/1/012021>.
- [23] A. Abbas, G.D. West, J.W. Bowers, P.M. Kaminski, B. Maniscalco, J.M. Walls, W.S. Sampath, K.L. Barth, Cadmium chloride assisted re-crystallization of CdTe: The effect of the annealing temperature, in: 2013 IEEE 39th Photovolt. Spec. Conf., IEEE, 2013: pp. 0356–0361. <https://doi.org/10.1109/PVSC.2013.6744166>.
- [24] S. Singhal, A.K. Chawla, H.O. Gupta, R. Chandra, Effect of annealing temperature and CdCl₂ treatment on the photo-conversion efficiency of CdTe/Zn_{0.1}Cd_{0.9}S thin film solar cells, *Bull. Mater. Sci.* 41 (2018) 159. <https://doi.org/10.1007/s12034-018-1658-3>.
- [25] T. Sinha, D. Lilhare, A. Khare, A review on the improvement in performance of CdTe/CdS thin-film solar cells through optimization of structural parameters, *J. Mater. Sci.* 54 (2019) 12189–12205. <https://doi.org/10.1007/s10853-019-03651-0>.
- [26] A. Romeo, E. Artegiani, CdTe-Based Thin Film Solar Cells: Past, Present and Future, *Energies* 14 (2021) 1684. <https://doi.org/10.3390/en14061684>.
- [27] I. Dharmadasa, A. Alam, How to Achieve Efficiencies beyond 22.1% for CdTe-Based Thin-Film Solar Cells, *Energies* 15 (2022) 9510. <https://doi.org/10.3390/en15249510>.
- [28] A. Paul, A. Singha, K. Hossain, S. Gupta, M. Misra, S. Mallick, A.H. Munshi, D. Kabra, 4-T CdTe/Perovskite Thin Film Tandem Solar Cells with Efficiency >24%, *ACS Energy Lett.* 9 (2024) 3019–3026. <https://doi.org/10.1021/acsenerylett.4c01118>.
- [29] J. Wang, M. Fang, G.T. Fei, M. Liu, G.L. Shang, L. De Zhang, Te hexagonal nanotubes: formation and optical properties, *J. Mater. Sci.* 51 (2016) 7170–7178. <https://doi.org/10.1007/s10853-016-9997-1>.
- [30] N.A. Shah, Z. Rabeel, M. Abbas, W.A. Syed, Effects of CdCl₂ Treatment on Physical Properties of CdTe/CdS Thin Film Solar Cell, in: *Mod. Technol. Creat. Thin-Film Syst. Coatings*, InTech, 2017. <https://doi.org/10.5772/67191>.
- [31] I.M. Dharmadasa, O.K. Echendu, F. Fauzi, N.A. Abdul-Manaf, O.I. Olusola, H.I. Salim, M.L. Madugu, A.A. Ojo, Improvement of composition of CdTe thin films during heat treatment in the presence of CdCl₂, *J. Mater. Sci. Mater. Electron.* 28 (2017) 2343–2352. <https://doi.org/10.1007/s10854-016-5802-9>.
- [32] I.M. Dharmadasa, Review of the CdCl₂ treatment used in CdS/CdTe thin film solar cell development and new evidence towards improved understanding, *Coatings* 4 (2014) 282–307. <https://doi.org/10.3390/coatings4020282>.
- [33] Z. Bai, D. Wang, Oxidation of CdTe thin film in air coated with and without a CdCl₂ layer, *Phys. Status Solidi* 209 (2012) 1982–1987. <https://doi.org/10.1002/pssa.201228107>.
- [34] X. Wang, J. Wang, M. Zhou, H. Zhu, H. Wang, X. Cui, X. Xiao, Q. Li, CdTe Nanorod Arrays on ITO: From Microstructure to Photoelectrical Property, *J. Phys. Chem. C* 113 (2009) 16951–16953. <https://doi.org/10.1021/jp905577u>.
- [35] K. Chi, Q. Li, X. Meng, L. Liu, H. Yang, Morphology-controlled synthesis and characterization of CdTe micro-/nanoscale structures by electrodeposition method, *J. Mater. Sci.* 52 (2017) 10431–10438. <https://doi.org/10.1007/>

s10853-017-1213-4.

- [36] A.S. Al-Kabbi, K. Sharma, G.S.S.S. Saini, S.K. Tripathi, Determination of the transport parameters of nanocrystalline CdSe:Cu thin films, *Phys. Scr.* 87 (2013) 025604. <https://doi.org/10.1088/0031-8949/87/02/025604>.
- [37] K.B.B. Chaudhari, N.M.M. Gosavi, N.G.G. Deshpande, S.R.R. Gosavi, Chemical synthesis and characterization of CdSe thin films deposited by SILAR technique for optoelectronic applications, *J. Sci. Adv. Mater. Devices* 1 (2016) 476–481. <https://doi.org/10.1016/j.jsamd.2016.11.001>.
- [38] D.N. Ahilfi, A.S. Alkabbi, K.A. Mohammed, K.M. Ziadan, Fabrication and Characterization of polyaniline/CdSe Device for Applications in Nano Structured Solar Cells, *IOP Conf. Ser. Mater. Sci. Eng.* 928 (2020) 072069. <https://doi.org/10.1088/1757-899X/928/7/072069>.
- [39] G.H. Tariq, M. Anis-ur-Rehman, Annealing effects on physical properties of doped CdTe thin films for photovoltaic applications, *Mater. Sci. Semicond. Process.* 30 (2015) 665–671. <https://doi.org/10.1016/j.mssp.2014.09.012>.
- [40] P.K.K. Kumarasinghe, A. Dissanayake, B.M.K. Pemasiri, B.S. Dassanayake, Thermally evaporated CdTe thin films for solar cell applications: Optimization of physical properties, *Mater. Res. Bull.* 96 (2017) 188–195. <https://doi.org/10.1016/j.materresbull.2017.04.026>.
- [41] A.A. Ojo, I.M. Dharmadasa, Factors affecting electroplated semiconductor material properties: The case study of deposition temperature on cadmium telluride, *Coatings* 9 (2019). <https://doi.org/10.3390/COATINGS9060370>.
- [42] A. Derbali, A. Attaf, H. Saidi, H. Benamra, M. Nouadji, M.S. Aida, N. Attaf, H. Ezzaouia, Investigation of structural, optical and electrical properties of ZnS thin films prepared by ultrasonic spray technique for photovoltaic applications, *Optik (Stuttg.)* 154 (2018) 286–293. <https://doi.org/10.1016/j.ijleo.2017.10.034>.
- [43] P. Hervé, L.K.J. Vandamme, General relation between refractive index and energy gap in semiconductors, *Infrared Phys. Technol.* 35 (1994) 609–615. [https://doi.org/10.1016/1350-4495\(94\)90026-4](https://doi.org/10.1016/1350-4495(94)90026-4).
- [44] R. Swanepoel, Determination of the thickness and optical constants of amorphous silicon, *J. Phys. E.* 16 (1983) 1214–1222. <https://doi.org/10.1088/0022-3735/16/12/023>.
- [45] K. Punitha, R. Sivakumar, C. Sanjeeviraja, V. Ganesan, Influence of post-deposition heat treatment on optical properties derived from UV–vis of cadmium telluride (CdTe) thin films deposited on amorphous substrate, *Appl. Surf. Sci.* 344 (2015) 89–100. <https://doi.org/10.1016/j.apsusc.2015.03.095>.
- [46] A. Guillén-Cervantes, M. Becerril-Silva, H.E. Silva-López, J.S. Arias-Cerón, E. Campos-González, M. Pérez-González, O. Zelaya-Ángel, Structural and optical properties of CdTe + CdTeO₃ nanocomposite films with broad blueish photoluminescence, *J. Mater. Sci. Mater. Electron.* 31 (2020) 7133–7140. <https://doi.org/10.1007/s10854-020-03284-z>.
- [47] R.S. Yavorskyi, Features of optical properties of high stable CdTe photovoltaic absorber layer, *Phys. Chem. Solid State* 21 (2020) 243–253. <https://doi.org/10.15330/pcss.21.2.243-253>.
- [48] M. Tarek El-Shahat, A.S. Ali, A.M. Hassana, E.S. Yousef, E.R. Shaaban, Performance-related structural, optical, and electrical characteristics of 2 μm the CdTe–CdSe absorption layer of solar cell, *J. Ovonic Res.* 19 (2023) 705–718. <https://doi.org/10.15251/JOR.2023.196.705>.
- [49] R. Swanepoel, Determination of surface roughness and optical constants of inhomogeneous amorphous silicon films, *J. Phys. E.* 17 (1984) 896–903. <https://doi.org/10.1088/0022-3735/17/10/023>.
- [50] S. Chander, M.S. Dhaka, Thermal evolution of physical properties of vacuum evaporated polycrystalline CdTe thin films for solar cells, *J. Mater. Sci. Mater. Electron.* 27 (2016) 11961–11973. <https://doi.org/10.1007/s10854-016-5343-2>.
- [51] A. Purohit, S. Chander, A. Sharma, S.P. Nehra, M.S. Dhaka, Impact of low temperature annealing on structural, optical, electrical and morphological properties of ZnO thin films grown by RF sputtering for photovoltaic applications, *Opt. Mater. (Amst.)* 49 (2015) 51–58. <https://doi.org/10.1016/j.optmat.2015.08.021>.
- [52] S. Chander, A. Purohit, C. Lal, M.S. Dhaka, Enhancement of optical and structural properties of vacuum evaporated CdTe thin films, *Mater. Chem. Phys.* 185 (2017) 202–209. <https://doi.org/10.1016/j.matchemphys.2016.10.024>.

- [53] Himanshu, S.L. Patel, A. Thakur, M.D. Kannan, M.S. Dhaka, Analysis of different annealing conditions on physical properties of Bi doped CdTe thin films for potential absorber layer in solar cells, *Sol. Energy* 199 (2020) 772–781. <https://doi.org/10.1016/j.solener.2020.02.066>.
- [54] A.M.A. Hakeem, H.M. Ali, M.M.A. El-Raheem, M.F. Hasaneen, Study the effect of type of substrates on the microstructure and optical properties of CdTe Thin Films, *Optik (Stuttg)*. 225 (2021) 165390. <https://doi.org/10.1016/j.ijleo.2020.165390>.
- [55] M.F. Hasaneen, W.S. Mohamed, Effect of CdCl₂ heat treatment in (Ar + O₂) atmosphere on structural and optical properties of CdTe thin films, *Optik (Stuttg)*. 160 (2018) 307–321. <https://doi.org/10.1016/j.ijleo.2018.01.112>.
- [56] A. Sharmin, S.S. Mahmood, M. Sultana, M.A.A. Shaikh, M.S. Bashar, Property enhancement of a close-spaced sublimated CdTe thin film by a post-growth activation step with CdCl₂ and MgCl₂, *Mater. Adv.* 5 (2023) 1205–1216. <https://doi.org/10.1039/d3ma00734k>.
- [57] K. Sharma, A.S. Al-Kabbi, G.S.S. Saini, S.K. Tripathi, Determination of dispersive optical constants of nanocrystalline CdSe (nc-CdSe) thin films, *Mater. Res. Bull.* 47 (2012) 1400–1406. <https://doi.org/10.1016/j.materresbull.2012.03.008>.
- [58] E.R. Shaaban, I.S. Yahia, N. Afify, G.F. Salem, W. Dobrowolski, Structural and the optical dispersion parameters of nano-CdTe thin film/flexible substrate, *Mater. Sci. Semicond. Process.* 19 (2014) 107–113. <https://doi.org/10.1016/j.mssp.2013.12.013>.
- [59] C. Kittel, Introduction to Solid State Physics Charles Kittel, (2005) 337–340.
- [60] D. Mergel, D. Buschendorf, S. Eggert, R. Grammes, B. Samset, Density and refractive index of TiO₂ films prepared by reactive evaporation, *Thin Solid Films* 371 (2000) 218–224. [https://doi.org/10.1016/S0040-6090\(00\)01015-4](https://doi.org/10.1016/S0040-6090(00)01015-4).
- [61] R.K.K.G.R.G. Kumarasinghe, P.K.K. Kumarasinghe, R.P. Wijesundera, B.S. Dassanayake, Thermally evaporated CdS/CdTe thin film solar cells: Optimization of CdCl₂ evaporation treatment on absorber layer, *Curr. Appl. Phys.* 33 (2022) 33–40. <https://doi.org/10.1016/j.cap.2021.10.011>.
- [62] M.S. R. Moghadam, M.H. Ehsani, H. Dizaji, No Title thickness dependence of structural and optical properties of CdTe films, *Iran, J. Mater. Sci. Eng.* 15 (2018) 21–31. <https://doi.org/https://doi.org/10.22068/ijmse.15.3.21>.
- [63] K. Punitha, R. Sivakumar, C. Sanjeeviraja, V. Sathe, V. Ganesan, Physical properties of electron beam evaporated CdTe and CdTe:Cu thin films, *J. Appl. Phys.* 116 (2014). <https://doi.org/10.1063/1.4903320>.
- [64] M.F. AL-Mudhaffera, M.A. Nattiqb, M.A. Jaberb, No Title Linear optical properties and energy loss function of Novolac: Epoxy blend film, *Arch. Appl. Sci. Res.* 4 (2012) 1731–1740.
- [65] Y. Harada, T. Kita, K. Matsuda, Y. Kanemitsu, H. Mariette, Near-field photoluminescence spectroscopy of CdTe/Cd 0.75 Mn 0.25 Te tilted superlattices, *Phys. Status Solidi C* 9 (2012) 262–265. <https://doi.org/10.1002/pssc.201100278>.
- [66] I. Riech, J.L. Peña, O. Ares, A. Rios-Flores, V. Rejón-Moo, P. Rodríguez-Fragoso, J.G. Mendoza-Alvarez, Effect of annealing time of CdCl₂ vapor treatment on CdTe/CdS interface properties, *Semicond. Sci. Technol.* 27 (2012) 045015. <https://doi.org/10.1088/0268-1242/27/4/045015>.
- [67] V. Venkatachalam, S. Ganapathy, I. Perumal, S. Devendrapandi, A. Ayyaswamy, State filling effects on photoluminescence and photovoltaic characteristic of aluminium-doped CdTe colloidal quantum dots stabilized in aqueous medium, *Chem. Pap.* 75 (2021) 1883–1892. <https://doi.org/10.1007/s11696-020-01406-9>.
- [68] H.N. Noori, A.F. Abdulameer, Study of optical and structural properties of CdTe quantum dots capped with 3MPA using hydrothermal method, *Chem. Methodol.* 6 (2022) 842–850.