

Research Paper

Effect of cathodic voltage on structural, optical, and surface properties of electrodeposition of CdZnTe thin film for optoelectronic applications

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Abstract

This study investigated the impacts of varying growth voltage on structural, optical, and surface characteristics of electrodeposited cadmium zinc telluride (CdZnTe) thin films. The electrodeposition was performed using a potentiostatic mode with a cheap two-electrode electrodeposition method. The production of the thin films took place at deposition voltages of 1700, 1750, 1800, and 1850 mV. X-ray diffraction (XRD), ultraviolet-visible (UV-Vis) spectroscopy, and scanning probe microscopy (SPM) were used to evaluate the features of CdZnTe thin films. The XRD analysis confirmed that polycrystalline cubic CdZnTe structures with (111) preferential orientation were detected. The maximum crystallite size, minimum dislocation density, number of crystallite sizes per unit area, and microstrain were recorded at 17500 mV growth voltage. The UV-Vis analysis revealed that the energy bandgap of CdZnTe thin films varied increased from 1.55 to 2.05 eV as the deposition voltage increased from 1700 to 1850 mV. Utilizing a cathodic voltage of 1750 mV, the highest average surface roughness measured was 52.15 nm. Thus, a deposition voltage of 1750 mV can be used as the optimized voltage for the growth of CdZnTe thin film, and it has potential applications for thin film-based solar cell devices.

1. Introduction

The attention in renewable and sustainable energy sources is growing worldwide due to increasing worries about the environment and the necessity of tackling the issue of climate change (Zyoud & Zyoud, 2024). To address the concerns of changes in climate, pollution of air and water, and others, a number of studies conducted in the last ten years suggested the use of green energy such as tides, wind, solar, geothermal, and hydropower (Solomon et al., 2024). However, availability is the

main limitation with these energy sources. Regarding to solar energy, the cost of producing solar panels is an obstacles to restricting its application (Ahmed et al., 2024a). To reduce the manufacturing costs and to increase solar panel conversion efficiency, thin film solar cells (TFSCs) hold great potential for future solar panel generation (Solomon et al., 2020).

TFSCs, which are composed of cadmium telluride (CdTe), are considered by the photovoltaic (PV)

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research community to be one of the most attractive possibilities because of their remarkable efficiency of energy conversion (22.1%) and their open-circuit voltage (OCV) exceeding 1.0 volt (Rahman *et al.*, 2020). Cadmium zinc telluride (CdZnTe) is a compound semiconductor group of II-VI, potentially having an energy bandgap engineering which suits specific application by generating a continuous sequence of solid CdTe and ZnTe. Zn-doped -CdTe thin films combine the properties of zinc with the unique characteristics of cadmium telluride, making them suitable for various applications, particularly in sensors (Shams *et al.*, 2020) and solar cells (Zyoud *et al.*, 2021). Introducing Zn on the CdTe lattice can enhance charge carrier mobility and overall device efficiency. These changes in bandgap energy influence the material's properties (Chaure *et al.*, 2008). The ternary compound CdZnTe has a bandgap that may be adjusted between 1.4 and 2.26 eV (Huda *et al.*, 2013).

In the past, several approaches have been employed to produce CdZnTe thin films, such as spray pyrolysis (Orletsky *et al.*, 2021), radio frequency (RF) sputtering (Huda *et al.*, 2013), close-spaced sublimation (Bie *et al.*, 2021), pulsed laser deposition (Liu *et al.*, 2013), chemical bath deposition (Trier, 2024; Surabhi *et al.*, 2022), and electrodeposition (Kathalingam *et al.*, 2021). For this study, electrodeposition was selected due to its advantages, such as low-cost and affordable instrumentation, excellent repeatability, high material consumption efficiency, rapid growth rate, and consistent deposition over large substrates (Bansal & Rajaram, 2005).

The quality of the film formed during the electrodeposition technique of thin film deposition is found to be highly dependent on several factors, including the number of ions in the electrolyte being deposited, duration, stirring, pH, the electrodes utilized, and the deposition voltage (Solomon *et al.*, 2018; Ahmed *et al.*, 2023b). Optimizing the deposition voltage has a major impact on the stoichiometric element's composition in the thin film electrodeposition technique. Optimizing film growth is the initial stage (Ahmed, *et al.*, 2024b). Especially, for CdTe, Te-rich *p*-type conductivity, and Cd rich *n*-type conductivity thin films are deposited at low and high deposition voltages, respectively (Ahmed *et al.*, 2023a).

Thus, when Zn is added to the CdTe lattice, the first step will be the optimization of deposition voltage for the formation of uniform and quality thin film.

The production of thin films in electrodeposition also significantly depends on the reduction potential. Because of what leaves as an electric field, ions in the electrolyte migrate in certain directions in the event that the electrodes get an electric potential (Solomon *et al.*, 2019). There are reports on the optimization of deposition voltage for the growth of CdZrS (Mohapi *et al.*, 2023), CdMnTe (Olusola *et al.*, 2020), CdZnS (Solomon *et al.*, 2019), and CdTe (Salim *et al.*, 2015). This work examines the impacts of varying growth voltage on structural, optical, and surface characteristics of electrodeposited CdZnTe thin films utilizing a low-cost, two-electrode method to form the thin layer on an FTO substrate. The weak salts of zinc acetate and cadmium acetate served as the precursors to Cd and Zn, respectively, to produce the CdZnTe thin films. The method applied is an inexpensive two-electrode electrodeposition that hasn't been documented yet.

2. Materials and Methods

In order to prepare the electrolyte solution array for the electrodeposition of CdZnTe thin films, 1.0 M of 98% pure cadmium acetate dihydrate [Cd(CH₃COO)₂·2H₂O] was utilized as the Cd source, 0.50 M of 98% pure zinc acetate dihydrate [Zn(CH₃CO₂)₂·2H₂O] as the Zn source, and 1 ml of 98% pure tellurium dioxide TeO₂ solution was utilized as the Te source. By using two-electrode electrodeposition procedures, the thin films were produced on a fluorine-doped tin oxide (FTO) substrate.

Before synthesis, the substrate was chopped into small pieces. After that, it was ultrasonically cleaned for 30 min using deionized water and a lab soap solution. Then, ethanol, acetone, and methanol were utilized for cleaning. Following washing, deionized water was used to clean the substrates, and they were then left to air dry. Ammonium hydroxide (NH₄OH) or a diluted solution of hydrogen chloride was applied to adjust the pH of the electrolyte bath to 3.00. During the synthesis procedure, the electrolyte bath's temperature was kept at 85 °C and moderately stirred using a magnetic stirrer.

A computerized Gill AC powered the system. The substrate was attached to a graphite rod and sealed with thread tape which was made of insulating

polytetrafluoroethylene (PTFE). This functioned as the working electrode, or cathode, while the anode, or counter electrode, was the graphite rod. Along with the 400 ml of deionized water, the Cd and Te sources were prepared, and then the Zn source was added. Conversely, 30 ml of diluted HCl solution was used to dissolve 2 g of TeO₂, and the mixture was mixed for 20 min to form the Te-containing solution. To preserve the uniformity of the zinc and Cd-containing solution, it was agitated for 5 h.

The solution was subjected to Cyclic Voltammetry (CV) studies to optimize the deposition voltage. The CV measurements show that the cathodic voltage between 1700 and 1850 mV has a good current density to form CdZnTe thin films. Within the range, 1700, 1750, 1800, and 1850 mV deposition voltages were chosen to the region where CdZnTe thin films were grown well. The conductive glass substrate that was previously cleaned and affixed to the working electrode was once finally washed with deionized water and submerged for 120 min. The samples were removed from the solution and dried in air. The grown samples were characterized by using X-ray diffraction (XRD), ultraviolet-visible (UV-Vis) spectroscopy, and scanning probe microscopy (SPM) for the structural, optical, and surface study, respectively.

The structural properties of electrodeposited CdZnTe were calculated by using equations 1 to 4. The Scherrer formula (equation 1) was used to determine the crystallite size (D) (Ahmed et al., 2024b; Ukarande et al., 2022; Mohapi et al., 2023).

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

where k is the Scherrer crystal shape constant (typically around 0.9, though it can vary depending on the shape of the crystallites), λ is the X-ray wavelength used in the diffraction (in nanometers), β is the full width at half maximum (FWHM) of the diffraction peak (in radians), and θ is the Bragg angle (in radians).

A measurement of the quantity of dislocations is the dislocation density (δ) in a crystal. It is calculated as the dislocation lines per crystallographic unit volume. The dislocation density can be estimated from XRD data, typically by using equation (2), in which D is crystallite

size (Hasan et al., 2023; Rahman et al., 2019; Ojo et al., 2021).

$$\delta = \frac{1}{D^2} \quad (2)$$

Micro-strain is a measure of the strain within a crystal lattice that arises from imperfections such as dislocations, lattice distortions, or other defects. In X-ray diffraction studies, micro-strain (ϵ) is often calculated using the broadening of diffraction peaks, which is given as equation (3) (Doroody et al., 2020; Ahmed et al., 2021; Ciris et al., 2021).

$$\epsilon = \frac{\beta_{hkl}}{4 \tan\theta} \quad (3)$$

where hkl denote the miller indices and β and θ are as given above. The number of crystallites per unit area (N) is commonly estimated using various techniques depending on the context, but one of the standard methods involves using the Scherrer equation (equation (4), in which D is crystallite size (Ahmed et al., 2023).

$$N = \frac{1}{D^3} \quad (4)$$

3. Results and Discussion

3.1 Structural properties

XRD was employed to analyze the structural characteristics of electrodeposited CdZnTe thin films. Figure 1(a) displays the XRD spectra of CdZnTe thin films produced at various voltages during deposition. The analysis results showed the detection of cubic phases with polycrystalline nanomaterials. The peaks are found at the angle of 24.10, 39.80, 46.97, and 62.80 with corresponding miller indexes of 111, 220, 311, and 331, respectively. There are peaks related to ZnTe at 31.00 and 33.26, which is a cubic structure at 420 and 422, respectively. These outcomes exhibited strong concurrence with Joint Committee on Powder Diffraction Standards (JCPDS) card no 752086 and 010582, respectively. Glass substrate (FTO)-related peaks were observed at 26.92, 34.08, 38.69, 51.88, 54.91, 61.89, and 66.56°. Because FTO is annealed at a greater temperature and has a more crystalline structure, its peaks are larger than those of films. The 111 preferential orientation peaks are utilized to estimate the structural parameters of CdZnTe.

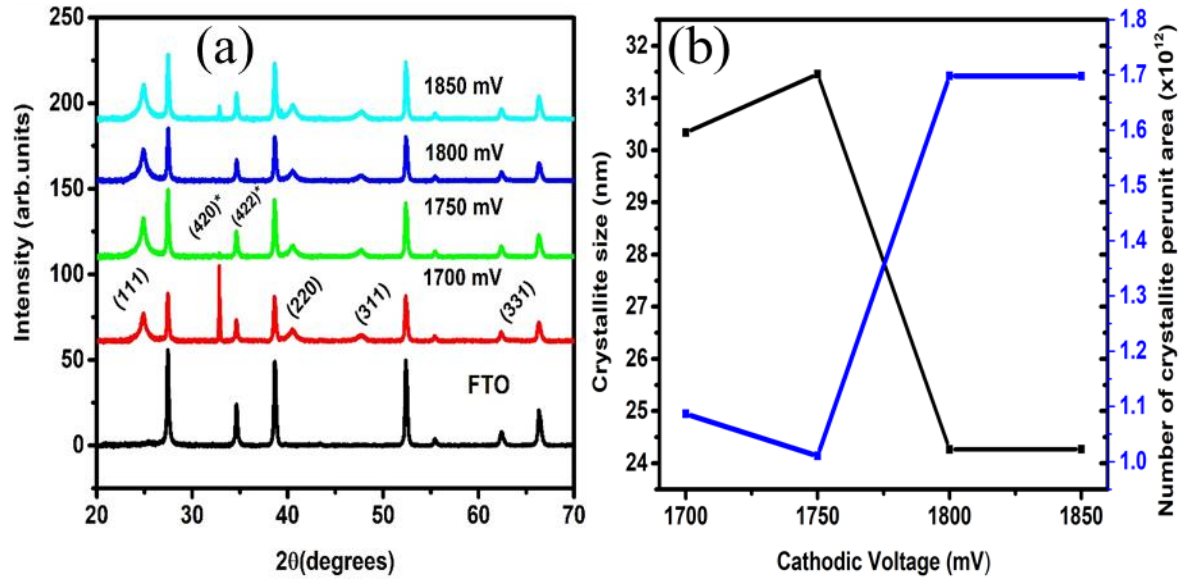


Figure 1: (a) XRD Spectra of CdZnTe deposited at different cathodic voltage and (b) the crystallite size (D) and number of crystallite per unit area (N) as a function of cathodic voltage

Figure 1 (b) shows that the D and N are functions of cathodic voltage. The D and N values were calculated by using equations 1 and 4, respectively. The maximum crystallite D of 31.6 was recorded at a deposition voltage of 1750 mV, whereas the minimum N of 1.01 was recorded at 1750 mV.

Figure 2(a) presents the peak intensity and FWHM as a function of cathodic voltage. The results confirmed that the maximum peak intensity and lowest FWHM were taken at the 1750 mV voltage of deposition. Figure

2 (b) shows the δ and ϵ as a function of cathodic voltage and the values were estimated by using equations 2 and 3, respectively. The results indicated that the lowest δ and ϵ documented at deposition voltage of 1750 mV. The lowest stain and dislocation show that the CdZnTe thin film is more crystallite and uniform. The overall analysis confirmed that the cathodic voltage of 1750 mV is taken as the optimized voltage in forming CdZnTe thin films for solar energy conversion applications.

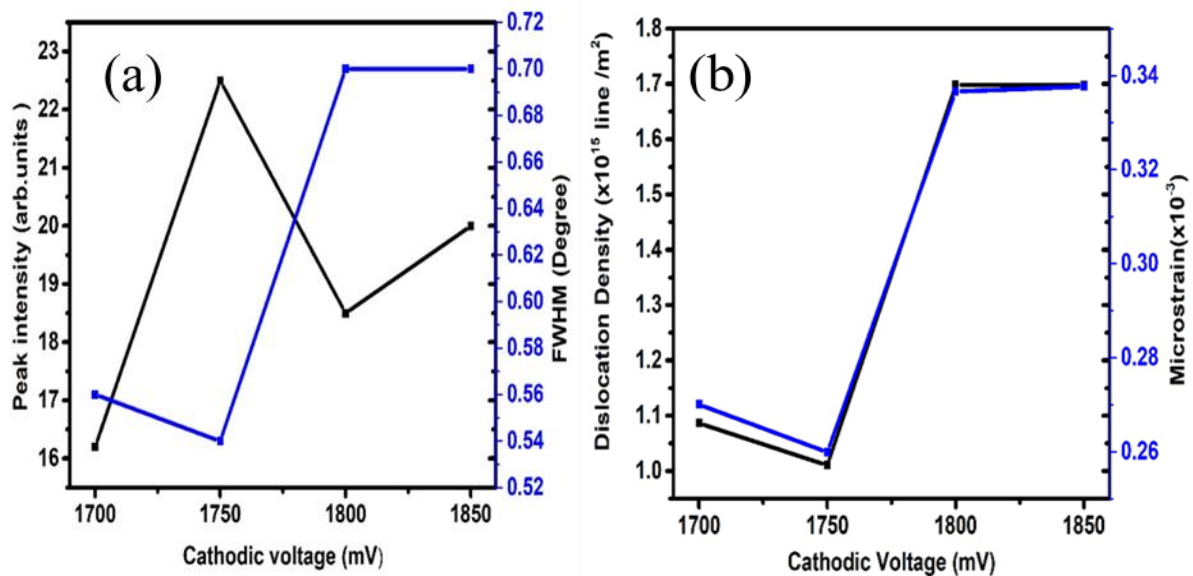


Figure 2: (a) peak intensity and full width at half maximum (FWHM) as a function of cathodic voltage and (b) dislocation density (δ) and micro-strain (ϵ) as a function of cathodic voltage

3.2 Optical properties

The optical properties of CdZnTe thin films are crucial for their applications in optoelectronics and photovoltaics. UV-Vis was utilized to examine the optical characteristics the formed CdZnTe thin films. Figure 3 (a) displays the wavelength-dependent absorbance spectra (nm). The optical absorbance was measured with a wavelength region of 300 – 1300 nm. The analysis depicted that there is a variation of absorbance with deposition voltage. The maximum near visible spectra region was noted at the 1750 mV voltage of deposition.

The absorbance squared (A^2) in conjunction with photon energy (eV) was displayed in Figure 3 (b). Bandgaps were obtained by extrapolating the straight-line section to the photon energy axis ($A^2 = \text{zero}$). The electrodeposited energy bandgap of the CdZnTe thin films was estimated from this investigation. The energy bandgap of CdZnTe thin films was documented as 2.05, 1.72, 1.55, and 1.55 eV with deposition voltages of 1700, 1750, 1800, and 1850 mV, respectively. The bulk bandgap of CdTe is 1.45 eV. Energy bandgap differences between CdTe and CdZnTe films ranged from 1.55-2.05 eV, showing continuous increase. The

increase in bandgap was due to the quantum confinement phenomenon decreasing in crystalline size and the addition of Zn-in CdTe caused by the deposition voltage.

3.3 Surface roughness properties

The surface properties of electrodeposited CdZnTe thin film were characterized by using SPM. Figure 4 shows the SPM image for electrodeposited CdZnTe thin films at various deposition voltages. SPM findings of this study showed the average surface roughness (R_a) properties of CdZnTe thin films to be 45.45, 52.15, and 47.12 nm, corresponding to deposition voltage of 1700, 1750 and 1800 mV, respectively.

From the analysis result, the films produced with a deposition voltage of 1750 mV are maximum, and a deposition voltage of 1700 mV is a minimum of 45.45 nm. The overall analysis showed that a deposition voltage of 1750 mV, which is the maximum crystallite size, optimum energy bandgap, and maximum average surface roughness, would be taken as the optimized voltage for the growth of CdZnTe thin films, which is used as an absorber layer in thin-film solar energy applications (Sharma et al., 2023).

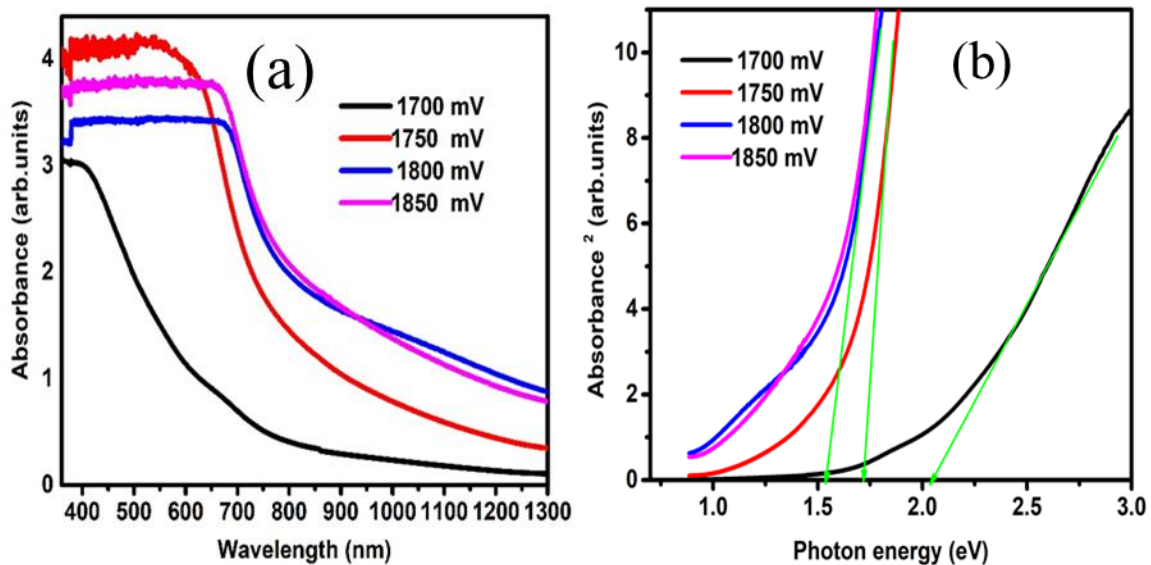


Figure 3: (a) Absorbance vs wavelength for CdZnTe thin film, (b) Absorbance square vs photon energy (eV)

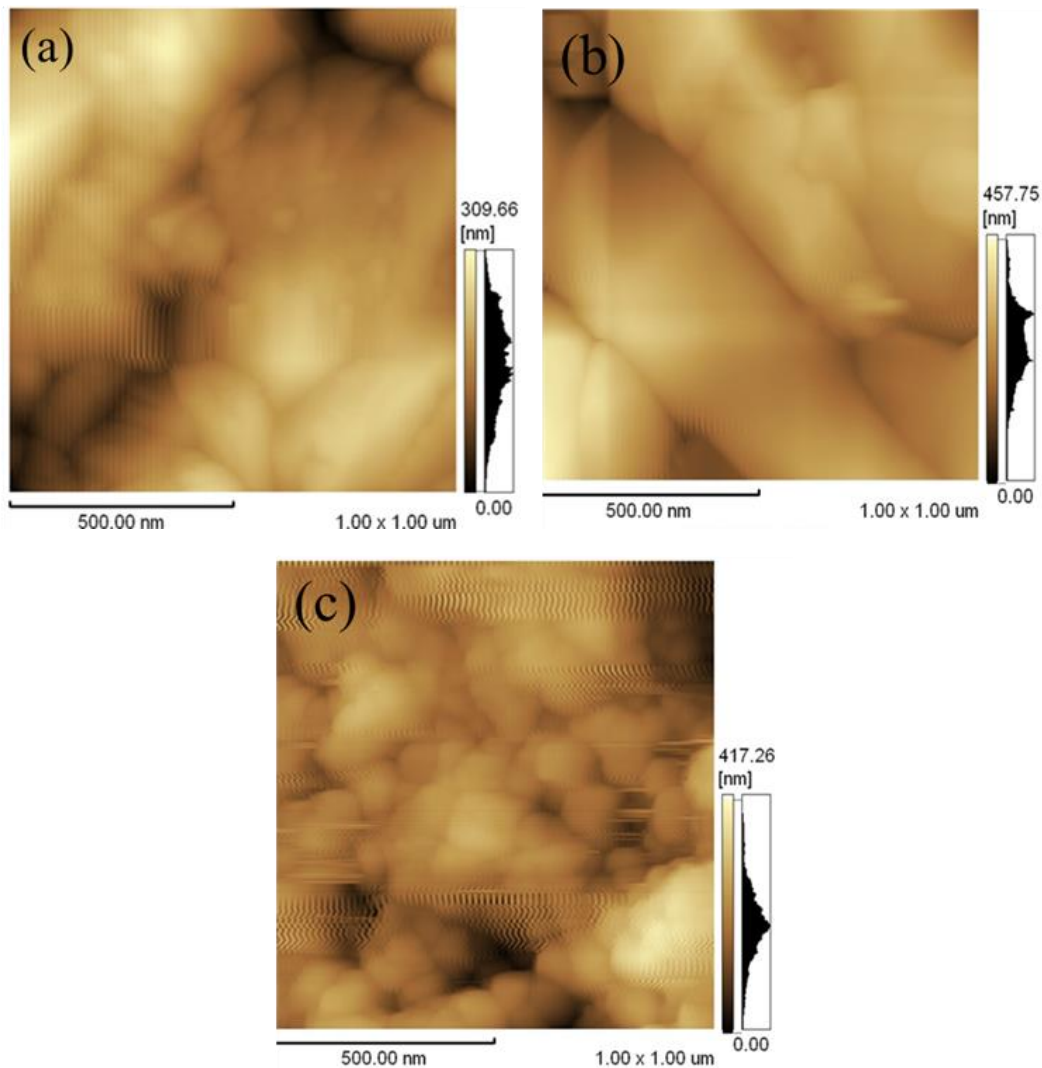


Figure 4: SPM image for Electrodeposited CdZnTe thin films at deposition voltages of (a) 1700 mV, (b) 1750 mV, and (c)1800 mV

4. Conclusion

A two-electrode electrodeposition method was utilized to effectively make CdZnTe thin film in potentiostatic mode with different deposition voltages for optoelectrical applications. The structural analysis showed the detection of the cubic phase CdZnTe thin films. The crystallite was maximum, maximum peak intensity, and low dislocation density and micro-strain were recorded at a cathodic voltage of 1750 mV. The energy bandgap for CdZnTe was 1.72 eV for 1750 mV

deposition voltage. The surface roughness was varied with cathodic voltage, and the maximum was recorded at 1750 mV. Thus, the CdZnTe thin film grown at a cathodic voltage of 1750 mV in this study can be considered for solar energy applications.

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