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Morphological, Optical, and Electrical Studies of PVD CdTe Thin Films for Photovoltaic Applications

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ABSTRACT

Nano-crystalline CdTe films were coated on glass and silicon substrates using the vacuum evaporation (PVD) technique, with annealing temperatures of 25, 100, 150, and 200 °C. This study aims to create a simple photoelectric cell using the effective light-absorbing layer CdTe as a thin film and Si as an n-type semiconductor. Additionally, it investigates the properties of CdTe thin films annealed at various temperatures. The following equipment was used: XRD, UV-visible spectrophotometer, SEM, and AFM. Moreover, the electrical characteristics of the fully designed devices were tested using I-V measurements and the Hall effect. Thin-film photovoltaics could become the primary source of global electricity. The CdTe thin films were coated using thermal evaporation. The best efficiency was 0.99% for the CdTe/Si structure with V_{oc} = 5.0 x 10^{-1} V, J_{sc} = 51.0 x 10^{-2} mA/cm^2, FF = 0.39, at 25 °C, and the efficiency decreased with increasing temperature. It has been found that annealing temperatures have an impact on the size of crystallites, the values of energy gaps, and the electrical properties of CdTe thin films.

Keywords: *CdTe films, electrical properties, optical properties, solar cells, thin films.*

1. INTRODUCTION

Cadmium telluride (CdTe) is an essential compound used in energy applications [1] and as a photocathode for water splitting [2]. CdTe films exhibit excellent electrical characteristics, making them favorable for solar energy applications.

CdTe has emerged as a highly successful competitor to silicon solar cell materials due to its good performance and cost-effectiveness in solar energy applications. Moreover, it boasts chemical robustness and stability, allowing for the fabrication of nano-layers using various deposition methods over large areas [3]. With a high absorption of optical radiation and an energy gap of 1.45 eV [4–6], CdTe holds promise for improving the efficiency of solar cells, which is a significant focus for researchers. In the past 5 years, researchers have made notable progress in enhancing CdTe cell efficiency. By reforming CdTe cells with a high-transparency n-layer, the efficiency was improved to 21.5% [7], further advancing to 22.1% [8]. CdTe can be synthesized as a thin film using physical or chemical methods. Various deposition techniques, such as laser ablation [9], electro-deposition, sputtering, spray pyrolysis, and thermal evaporation [10], can be employed to prepare CdTe films. Among these methods, thermal evaporation stands out for its high deposition rate, low material consumption, and cost-effectiveness. CdTe powder is evaporated from heated crucibles at a vacuum of 10^{-5} mbar onto glass or metal substrates.

Multi-layer structures are prepared using different techniques, categorized into high- or low-temperature procedures, and have a thickness of 2 x 10^{-6} µm [11, 12]. CdTe coatings may be polycrystalline or single-crystalline, influencing their properties [13]. It is important to note that the performance of a CdTe solar cell can be significantly influenced by both junctions (emitter or collector) [14]. This article aims to design a simple photoelectric cell using the effective light-absorbing layer CdTe as a thin film deposited by the PVD method on a-Si as an n-type semiconductor. It also investigates the characteristics of CdTe thin films annealed at different temperatures.

2. METHODOLOGY

The CdTe films were fabricated using the thermal evaporation deposition (PVD) method, coating them onto glass and silicon slides. The substrate cleaning process involved washing with Deionized (DI) water and soap for 5 minutes, followed by a 15-minute acetone wash and rinsing with DI water. Before the deposition process, the chamber was evacuated for about 1.5 hours using rotary and diffusion pumps, with the voltage adjusted accordingly. CdTe powder was then placed in a heated boat made of molybdenum material. The vacuum pressure was set at 1.5×10^{-4} mbar, and an 80 V was applied to the crucible boat to evaporate the CdTe powder onto the substrate. The prepared films were subsequently annealed at temperatures of 25, 100, 150, and 200 °C.

Structural properties, including lattice constants, were determined for the cubic structure [15]. The dislocation density (δ) was determined using Smallman's relation [16], and the specific surface area (SSA) was calculated as SSA = 6000/(D.ρ), where D is the crystallite size and ρ is the density of CdTe (5.85 g/cm^3) [17]. The band gap of the CdTe nanostructures was also determined [18, 19]. The electrical properties of the CdTe-coated glasses were studied by creating aluminum (Al) electrodes using the thermal evaporation method, with a certain distance between them. The current-voltage (I-V) test was performed to describe the effect of heterojunction; the output current depends on the applied voltage, and when applied dark current-voltage will produce forward and reverse biases. Hall Effect measurements were also done by Van der Pauw (Ecopia HMS-3000) Systems.

Free charges are deflected by an external magnetic field, thus creating a Hall potential. The sign of the Hall coefficient (RH) determines the type of charge carrier; if it is negative, this means the charge carrier electrons and the semiconductor are n-type. When positive, the charge carrier hole and the semiconductor are p-type. On a thin layer of CdTe, aluminum electrodes are deposited using thermal evaporation, a special mask, on the surface of the sample. Four points are created in the corners, usually measuring (1 x 1) cm^2, and used as contacts. Then, the sample is connected to an electrical circuit, and a magnetic field is applied perpendicular to the sample. After that, the continuous current and the Hall voltage (VH) are measured. To assess the efficiency of the solar cell, incident light, short-circuit current, fill factor, and open-circuit voltage were taken into consideration [20]. Overall, the text appears to be well-structured, and the revised version aims to enhance clarity and understanding for the readers.

3. RESULTS AND DISCUSSION

3.1 Structural Characteristics

CdTe films were examined using X-ray diffraction (XRD), and the results are presented in Figure 1. The obtained patterns indicate a cubic structure (No. file 9008841) with an F-43m space group. The angles 23.75, 39.28, 46.44, and 62.41 correspond to the Miller indices (111), (202), (311), and (313), respectively. The dominant pattern observed is (111), suggesting that the films have an ideal orientation. Furthermore, with increasing annealing temperature, the intensity of the (111) pattern increases, indicating an improvement in the crystallinity of the CdTe films. The Scherrer equation is particularly useful for estimating the particle size of the CdTe film [21, 22]. All the collected data have been tabulated in Table 1.

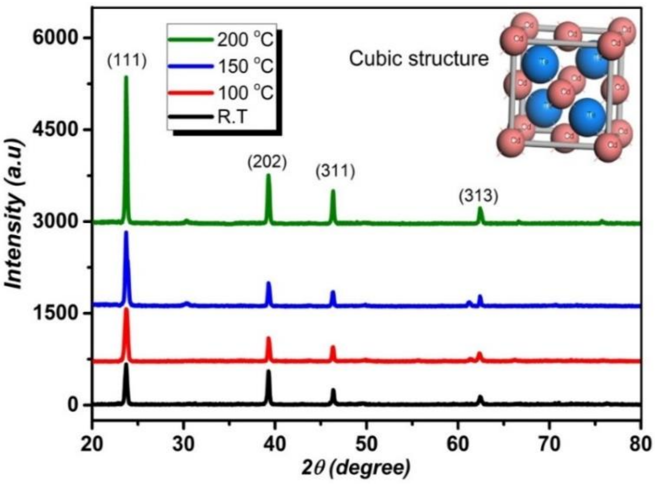

Figure1 XRD peaks of CdTe thin films.

The higher temperatures used during the annealing process have resulted in larger crystallites, crystals, and cell volumes in the CdTe films [23]. This can be attributed to thermal expansion and a faster rate of growth at elevated temperatures. As shown in Figure 2a, an interesting observation was made regarding the lattice constants. With an increase in cell volume, the lattice constants also increase. Additionally, it was noted that as the annealing temperature increased, the film thickness also increased. This phenomenon can be explained by the influence of high temperatures on grain boundaries, promoting their movement and leading to the coalescence of additional grains. As a result, the average grain size and surface roughness increase. The revised provides a more concise and coherent description of the impact of annealing temperatures on the CdTe films, their crystallites, and lattice constants, when. Increasing the temperature to 200 C° leads to increased stress on the surface of sample, as the particle size increases with temperature, so the dislocation density decreases, which causes a decrease in cell volume and lattice parameter.

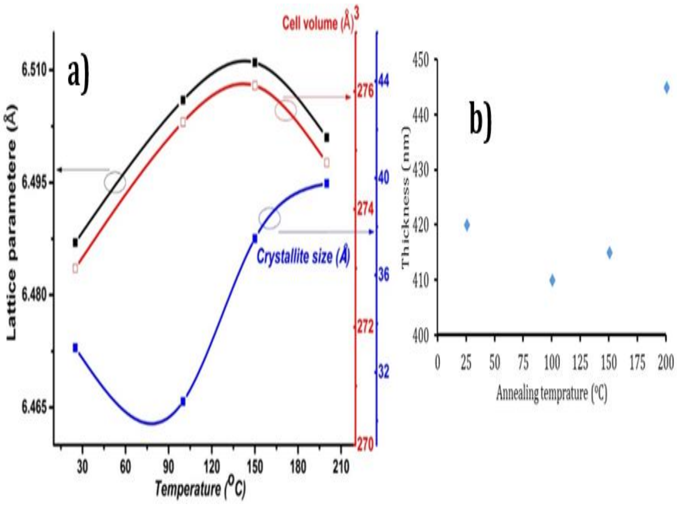

Figure 2 a. Relation between lattice parameter, cell volume, and crystallite size as a function of annealed temperature. b. the thickness of CdTe films at different temperatures

3.2 Electrical test

3.2-1 I-V test

Figure 3 illustrates the variation in resistivity, mobility, and conductivity of CdTe films. It is evident that the resistivity initially increases and then decreases, exhibiting an inverse relationship with both mobility and conductivity. As the annealing temperature increases, the films demonstrate a reduction in resistivity, attributed to the enhanced fluidity of electron carriers with increasing crystallite size. Consequently, the conductivity and mobility also increase with rising temperatures, as indicated in Table 2 [24]. The data in Figure 3 and Table 2 highlight the important role of annealing temperature in influencing the electrical properties of the CdTe films.

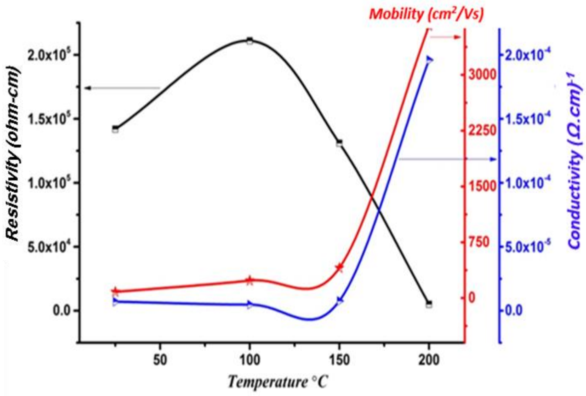

Figure 3 The relation between ρ, σ_c, and mobility as a function of temperature degree

Table 1 The values of lattice constants, cell volume, D, δ, SSA, packing density, and angles in degrees.

Specimen Temp. °C	a=b=c (Å)	Cell volume (Å^3)	Crystallite size (Å) Scherrer Eq.	Dislocation density (Lines/m^2)*10^{16}	SSA (m^2/g)	Packing density	Angles (α, β, γ) in degree
R.T.	6.487	273.00	33.01	9.17	310.7	0.911	90
100	6.506	275.48	30.79	10.54	333.1	1.144	90
150	6.511	276.10	37.51	7.10	273.4	1.043	90
200	6.501	274.79	39.78	6.31	257.8	0.872	90

Table 2 The values of resistivity, mobility, conductivity, energy gap, and thickness.

Temperature degree (°C)	Resistivity (Ω.cm)	Mobility cm^2/Vs	Conductivity (Ω.cm)$^{-1}$	Energy gap (nm)	Thickness (nm)
R.T.	6.487	273.00	33.01	9.17	310.7
100	6.506	275.48	30.79	10.54	333.1
150	6.511	276.10	37.51	7.10	273.4
200	6.501	274.79	39.78	6.31	257.8

Figure 4 presents the variations in reverse current with temperatures of 25 °C, 100 °C, 150 °C, and 200 °C. It is noteworthy that the reverse current exhibits a notable increase at 150 °C. This phenomenon can be attributed to an increase in the emission of electron-hole pairs within the depletion region, resulting in an elevation of the minority carrier concentration at this temperature. The changes in reverse current observed in Figure 4 can be attributed to the impact of temperature on the behavior of electron-hole pairs in the depletion region, elucidating the temperature-dependent behavior of the CdTe films.

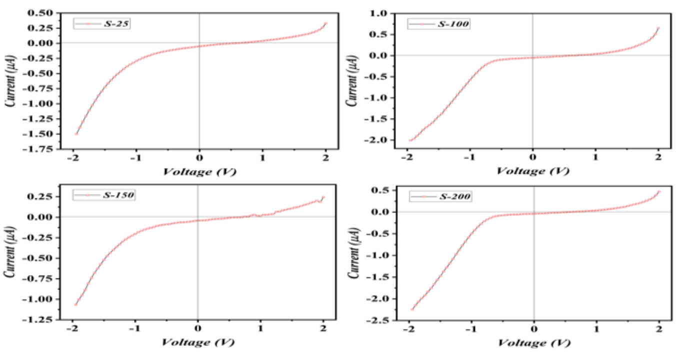

Figure 4 I-V test for CdTe film

3.2-2 Hall Effect

The conductivity type and Hall mobility (μH) of the thin films annealed at 25 °C, 100 °C, 150 °C, and 200 °C were determined through Hall measurements, as presented in Table 2. It is evident from Table 3 that all films demonstrate p-type conductivity. This conclusion is based on the positive Hall coefficients observed in all prepared films, indicating that holes are the majority charge carriers involved in the conduction process, confirming the p-type conduction of the CdTe films. The Hall measurements provided valuable insights into the electrical characteristics and charge carrier types of the CdTe thin films annealed at different temperatures.

Table 3 Hall coefficients measurement of the thin films annealed temperature at 25 °C, 100 °C, 150 °C, and 200 °C.

Temperature degree (°C)	Hall coefficient	Type
25	2.903×10^7	P
100	4.976×10^7	P
150	1.171×10^7	P
200	5.313×10^7	P

3.3. Solar Cell Characteristics

3.3-1 Fill Factor and Cell Efficiency

The efficiencies of the CdTe/Si structure were calculated at annealing temperatures of 25 °C, 100 °C, 150 °C, and 200 °C, as summarized in Table 4. The optimal efficiency was achieved at 25 °C with Voc = 5.0 x 10^{-1} V, Jsc = 51.0 x 10^{-2} mA/cm^2, and a fill factor of 0.39. However, as shown in Figure 5, the efficiency decreased with increasing temperature. The parameters such as open-circuit voltage (Voc), short-circuit current density (Jsc), and fill factor exhibited slight changes between increase and decrease as the temperature rose. This behavior can be attributed to the effect of the band gap of the optoelectronic materials used in solar cell design on the reverse saturation current density, which decreases with increasing temperature, as indicated in Table 4. The observation of efficiency variations with temperature emphasizes the significance of annealing temperature in influencing the performance of the CdTe/Si structure solar cell. It also highlights the impact of temperature on the optoelectronic properties of the materials, which should be considered for the design and optimization of solar cells using CdTe films.

Table 4 Solar cell characteristics

Temperature degree (^{o}C)	25	100	150	200
Area (cm^2)	1	1	1	1
Thickness (nm)	450	410	415	445
J_{SC} (mA/cm^2)	0.51	0.50	0.51	0.38
V_{OC} (V)	0.50	0.55	0.60	0.55
J_{max} (mA/cm^2)	0.32	0.30	0.26	0.28
V_{max} (V)	0.31	0.32	0.36	0.33
F.F	0.39	0.35	0.39	0.44
Efficiency (%)	0.99	0.96	0.93	0.92

Figure 5 illustrates the variation of current density with voltage at different temperatures for the Al/p-CdTe/n-Si/Al solar cell structure. The electrical parameters of the solar cell components are presented in Table 4. As observed from the table, with an increase in the annealing temperature of the CdTe films, the short-circuit current density (Jsc), voltage (Voc), and fill factor (FF) initially increase and then decrease. However, the efficiency of the solar cell decreases as the annealing temperature is raised. This trend may be attributed to structural changes occurring in the CdTe film material during the annealing process at higher temperatures. The variations in the electrical parameters and efficiency emphasize the sensitivity of the solar cell's performance to the annealing temperature and the importance of optimizing this parameter for achieving the highest efficiency in the Al/p-CdTe/n-Si/Al solar cell structure. It is crucial to carefully control the annealing process to ensure the desired properties and efficiency of the CdTe thin films in the solar cell design [25].

3.4 Optical studies

CdTe films were tested by UV-visible spectroscopy to study their optical properties [26]. Figure 6 demonstrates the transmission of the films at different temperatures. All the samples have shown good transmittance at wavelengths greater than 800 nm.

The growth process of CdTe films affects the crystal structure and leads to changes in the band gap. Figure 7 exhibited the energy gap curves of CdTe films. The figure was plotted by (hυ) and (αhυ)2 on (x-y- axes) respectively. The band gap was estimated by putting a line to the value of hυ with zero absorption coefficients (α). The growth process of CdTe films affects the crystal structure and leads to changes in the band gap.

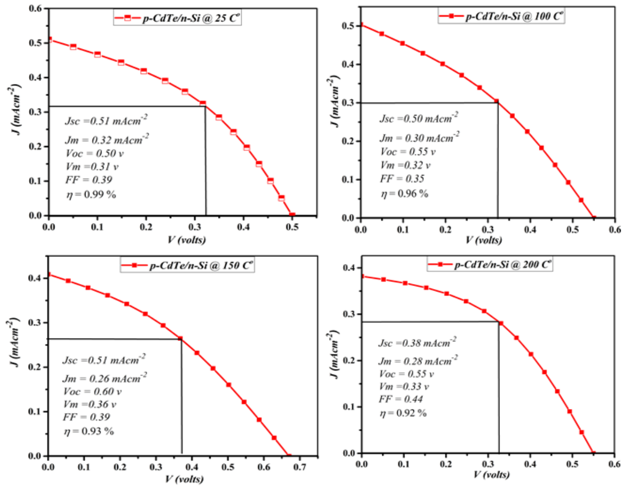

Figure 5 Al/p-CdTe/n-Si/Al Solar cells performance

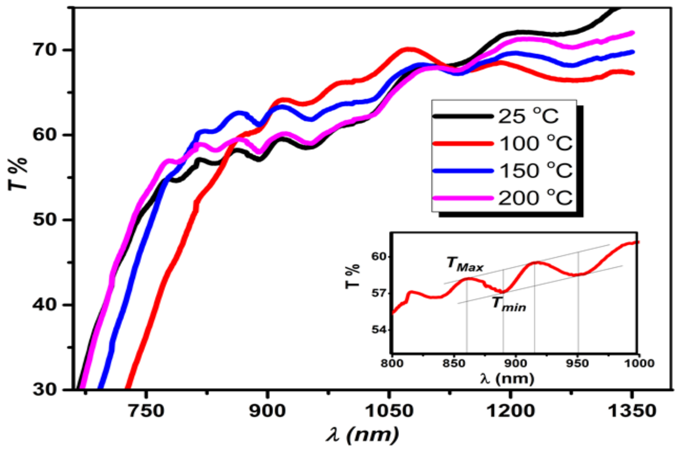

Figure 6 Shows the relation between the transmission of CdTe thin film and wavelength.

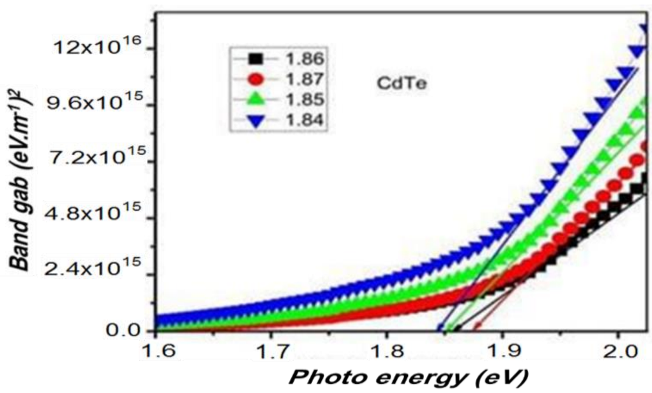

Figure 7 Tauc plot of deposited CdTe thin films annealed at different temperatures.

Figure 8 presents the variations in the energy band gap (Eg) of CdTe films at different temperatures. The measured values of Eg were 1.86, 1.87, 1.85, and 1.84 eV, and these data are compiled in Table 2. In general, the energy gap of a semiconductor is influenced by temperature. At (-273°C) temperature, the conduction band remains empty, and all electrons are present in the valence band. As the temperature increases, there is an impact on the energy difference between these two bands, resulting in the narrowing of the energy gap. Therefore, as the temperature rises, the energy gap of the CdTe films decreases, leading to changes in their optical and electrical properties. The analysis of energy band gap variations with temperature is crucial for understanding the behavior of CdTe films and optimizing their performance for various optoelectronic applications.

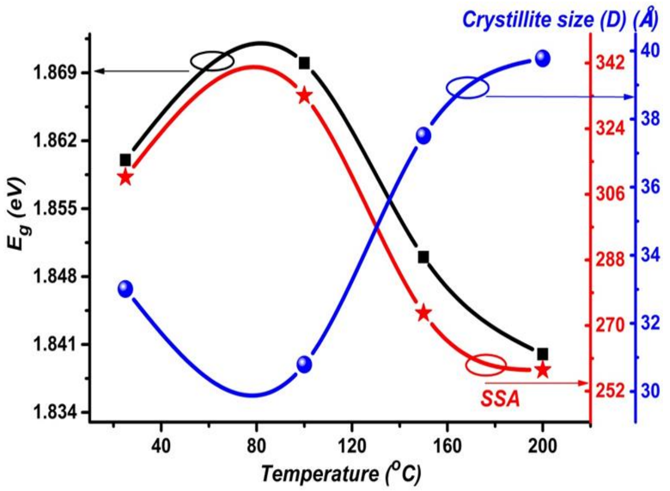

Figure 8 Relation of the energy gap of CdTe among the Crystallite (D) size and the specific surface area (SSA) at the different annealed temperatures.

3.5 Thickness determination

The thickness of the films is calculated by the Swanepoel method, which has proven to be a reliable approach for calculating the optical constants of thin films. This method is particularly effective when the transmittance spectrum of the film exhibits wavelike patterns resulting from the reflection of the probe beam at different interfaces [27]. All data are tabulated in Table 2.

3.6 Fourier Transform Infrared Radiation (FTIR)

The FTIR spectra were used to gain further insights into the nature of the bonds and the structure of the CdTe films manufactured at different temperature levels. Figure 9 shows the FTIR spectrum of the CdTe films, and it is evident that all spectra of pure CdTe nanocrystals exhibit almost similar peaks in various bands. Specifically, the peaks observed between 3860 and 3200 cm^{-1} correspond to (O-H) stretching vibrations. The absorptions at 2885 and 2966 cm^{-1} are attributed to the single bond (C-H) vibrations, specifically CH3 and CH2 groups. The peaks at 2264 and 2117 cm^{-1} correspond to the CC stretching triple bond. The wider absorption observed at 1689 cm^{-1} is associated with the C=C double bond. The longest absorption peak at 1527 cm^{-1} corresponds to a symmetric vibration related to the (NO) group. Peaks between 1273 and 1150 cm^{-1} are the result of (C-H) wag stretching. FTIR spectra are particularly sensitive to (C) and (O2) bonding, hence the peak at 1384 cm^{-1} corresponds to COO groups, indicating ligand stretching [28, 29]. The analysis of the FTIR spectra provides valuable information about the chemical bonds and functional groups present in the CdTe films, shedding light on their structural characteristics. The FTIR results are essential for understanding the material's composition and properties, especially as it relates to the annealing temperature during the manufacturing process.

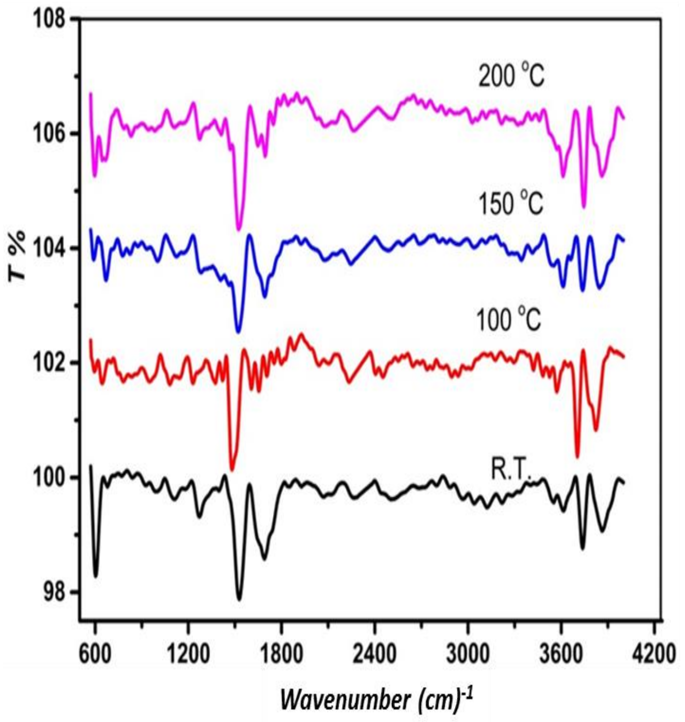

Figure 9 FTIR spectra of CdTe thin films

3.7 Atomic Forces Microscopy (AFM)

From Figure 10, it is evident that the first sample annealed at 25°C exhibited the highest thickness of the outer layer, measuring 10.3 nm. Additionally, the root mean square roughness was relatively small, with a value of 0.67 nm. The small root mean square value and grain size indicate a good crystalline structure, and the crystals appear to be evenly distributed throughout the film. However, as the annealing temperature increased to 100 °C, 150 °C, and 200 °C, the root mean square roughness also increased significantly, measuring 0.78 nm, 1.66 nm, and 9.98 nm, respectively. Similarly, the highest thickness increased from 19.9 nm to 40.6 nm as the annealing temperature rose. This suggests an increase in surface roughness due to the crystallization process occurring at higher temperatures. The changes in thickness and root mean square roughness with increasing annealing temperatures indicate alterations in the film's crystalline structure and surface characteristics. The increasing roughness at higher temperatures may have implications for the optical and electrical properties of the CdTe films, particularly in applications such as optoelectronics and solar cells. The findings from Figure 10 offer valuable insights into the relationship between annealing temperature, film morphology, and its potential impact on device performance and functionality.

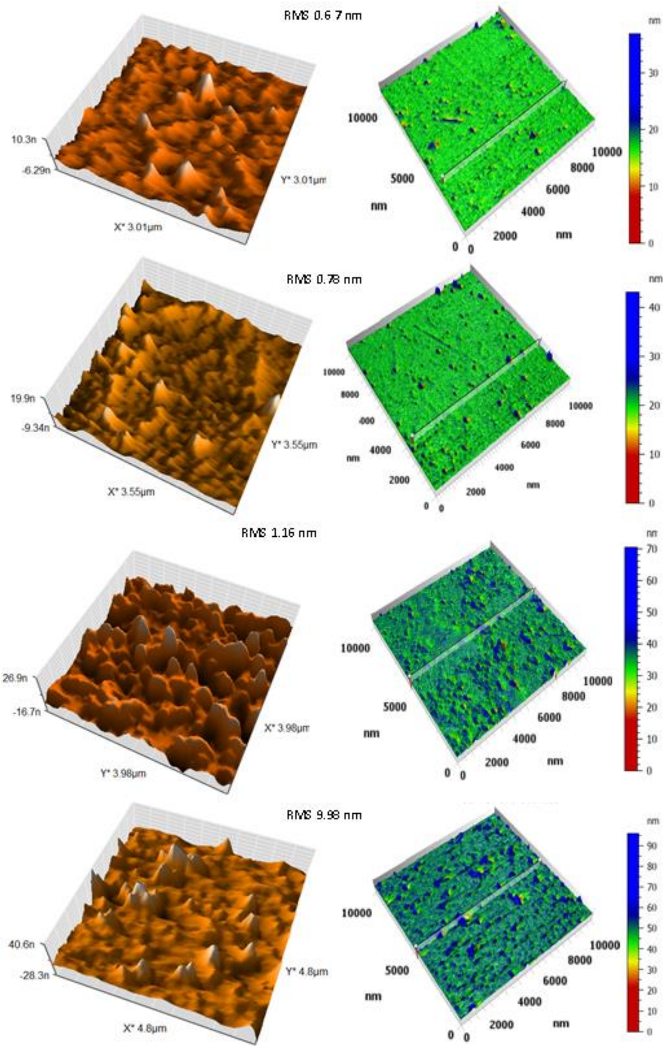

Figure 10 AFM of CdTe samples annealed at 25, 100, 150, and 200 °C from up to down.

4. CONCLUSION

The promotion of clean energy usage is crucial as it is environmentally friendly and contributes to reducing carbon emissions, addressing the challenges the world may face in the future, such as the depletion of fossil fuels. In this study, the PVD technique was employed to create nanostructured CdTe films. The examination of CdTe films by XRD revealed a cubic structure, with the crystallite size increasing with temperature in the range of 150 °C to 200 °C. Additionally, the volume of the unit cell for CdTe thin films was presented. The optical characteristics of the films exhibited good transmittance when tested with UV-visible radiation. The transmittance curves showed fringes, indicating increased light absorption. The refractive index, a significant property, was investigated and found to decrease as a function of wavelengths in this work. The study thoroughly discussed the variation in particle size and its correlation with band gaps, specific surface area (S.S.A.), electrical characteristics, and their interrelationships. The surface topology displayed very smooth particles, and collectively, these properties suggested that the CdTe films prepared were suitable for photoelectric cell applications. Overall, this research highlights the potential of CdTe thin films as promising materials for clean energy applications, particularly in photoelectric cells, and contributes to the understanding of their structural, optical, and electrical properties. Emphasizing and advancing such clean energy technologies can play a vital role in mitigating environmental challenges and fostering sustainable development.

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