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Development of Some Physical Properties of Cadmium Telluride Coatings Prepared by Spray Pyrolysis

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Abstract

For this work, the spray pyrolysis technique is employed to create uniform thin films of cadmium telluride (CdTe) at 350°C on glass substrates. For optical and structural examination, the films that were deposited undergo annealing at 573 K and 723 K. In an air atmosphere, before being examined using an XRD, a microscopy force atomic (AFM), and UV-Vis spectrophotometer. The film's cubic structure and polycrystalline nature were demonstrated by the XRD tests with preferred orientation (111), and temperatures for annealing improve crystalline speed. Crystallite size and microstrain were among the microstructural metrics that were computed with an increase in annealing temperatures; it was found that the microstrain decreased and the crystallite size increased. In the transmittance's strong absorption region, the basic optical parameters, including the band gap and absorption coefficient, were computed. The optical transition in these coatings was discovered to be a direct transfer, while the energy band gap is shown to decrease with annealing, while increases in optical absorbance.

Keywords: Physical characteristics, Spray pyrolysis technique, Cadmium telluride.

1. Introduction

Cornerstone material in various applications within electronic and optoelectronic devices. Compared with alternative semiconductor compounds, it has the highest ionic character, the least negative formation enthalpy, the largest lattice parameter, the lowest melting temperature, and a high atomic number (1–3). The direct band gap of CdTe, an II-VI perfect semiconductor (4, 5), is 1.45 eV, and its crystal structure is zinc blende (cubic) (6–8). Techniques for thin-film deposition have been used to create p-type CdTe films. of high quality, suitable for solar cell applications. These techniques include electrochemical deposition (9), closed-space sublimation (CSS) (10), chemical spray pyrolysis (3, 11), and physical vapor deposition (12).

Vacuum evaporation (13, 14), vapor transport deposition (15), screen printing, MOCVD stands for metal-organic chemical vapor deposition (16–18), and radio frequency (RF) sputtering (5, 19, 20). When combined with a CdS window layer of the n-type, these films have achieved solar cell conversion efficiencies of up to 16% (5). The chemical spray pyrolysis (CSP) technique stands out as a highly efficient approach for the deposition of polycrystalline films throughout a variety of materials. This research aims to enhance the structural and optical properties by increasing the absorption spectrum of the prepared films, making them suitable for optoelectronic applications, especially in the field of clean energy.

2. Materials and Methods

The process of spray pyrolysis was employed to produce cadmium telluride, as shown in **Figure (1)**. To manufacture CdTe films, 0.05 M precursor solutions of $CdCl_2$. H_2O in 25 ml of purified water and TeO_2 in 20 ml of solution of ammonia, 2 ml of Hydrochloric Acid, and 3 ml of hydrazine hydrate was produced. The first two solutions are combined (21). The CdTe films, which had a thickness of about 550 nm, the distance between the nozzle and the substrate was equal to 24 cm, and a spray rate of 0.167 ml/sec, were deposited on glass substrates slide of (2×2.5 cm) that had been extensively cleaned at 350 °C. The films were allowed to spontaneously cool to ambient temperature following deposition. The CdTe film was annealed for an hour at two distinct temperatures (573 and 723 K). Diffraction of X-rays (XRD) has been used to analyze the structural characteristics.

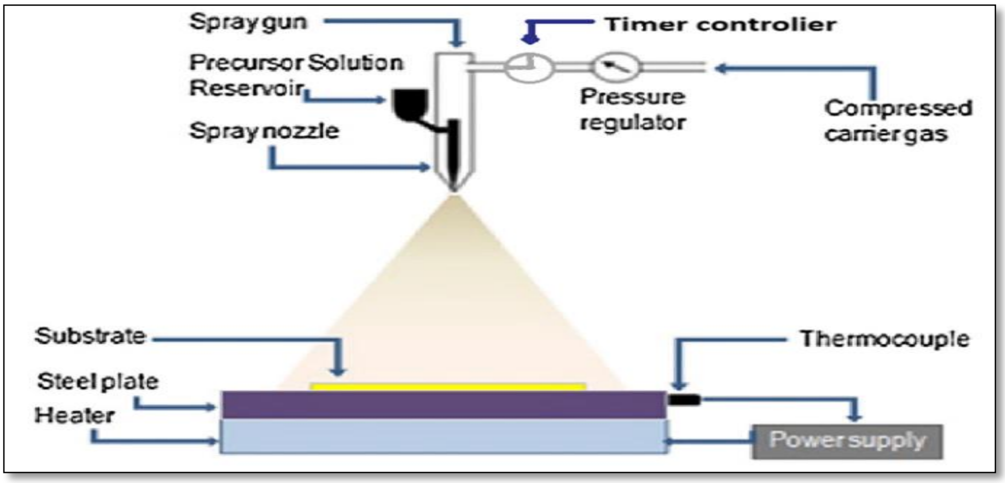

Figure 1. Experimental setup schematic for spray pyrolysis method (23)

3. Results and discussion

3.1. Structural analysis

Figure (2) shows the X-ray diffraction (XRD) patterns of CdTe coatings at different annealing temperatures for the films. According to reference code (03-065-0880), the XRD data showed that all deposited films formed a polycrystalline structure with a cubic crystal structure. for every thin film of CdTe, three peaks that correspond to the reflection planes of (111), (220), and (311) were found at 23.92°, 39.24°, and 46.39°, respectively. Additionally, **Figure (2**) shows that when the film is annealed, the peak intensity improves, and the plane of orientation that is preferred by (111) increases. This could be because the thin films' degree of crystallinity increased along the preferred orientation plane (111) with rising annealing temperature. Following the application of the Scherrer equation to get the crystallite size (D), the dislocation density (δ), and strain on a lattice (ε), respectively (23–25).

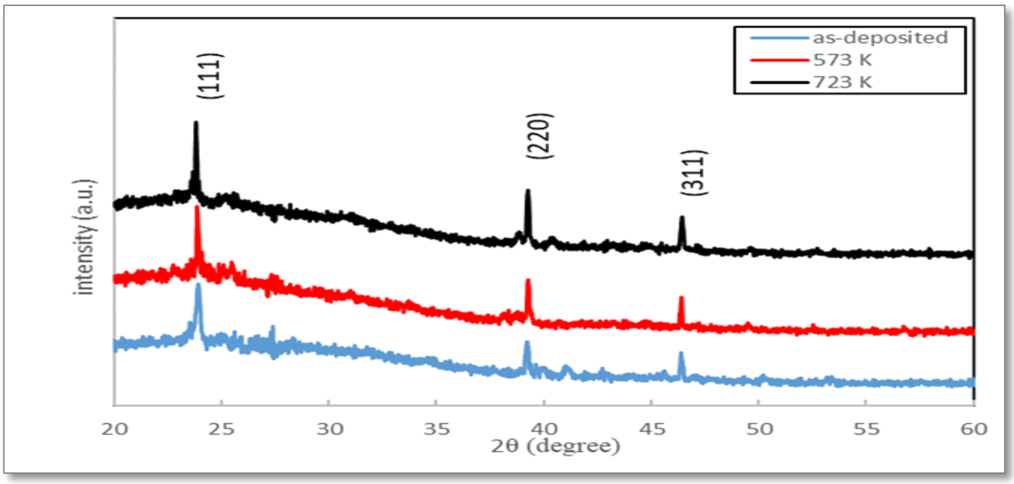

Figure 2. The XRD patterns of thermally annealed and as-deposited CdTe thin films

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

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

$$\varepsilon = \frac{\beta \cos\theta}{4} \quad (3)$$

where β is the FWHM, K is a constant (≈ 0.9), and λ (0.154 nm) is the length of the beam of the X-ray source.

Table (1) displays the microstructural features, such as the size of the crystallites (D), dislocation densities (δ), and strain of the lattice (ε) that were determined on the (111) plane. **Table (2)** presents the crystallite size estimated using Scherer's equation. The results indicate that the CdTe sample at 723 K has the largest crystallite size compared to the other samples. This is attributed to the decrease in the full width at half maximum (FWHM), which contributes to the increase in crystallite size of these films (see equation Scherrer formula), and according to the Scherrer formula, an average-sized crystallite was 30 nm. The decreasing in microstrain and dislocation density with increasing annealing temperatures (573&723) K. This is due to the direct proportionality between microstrain and FWHM of the main peak and the inverse proportionality between the dislocation density and the crystallite size, and these values are in good agreement with terms that have been previously reported (26).

Table 1. Parameters (CdTe) film X-ray diffraction at different temperatures.

Annealing Temperature	2θ(deg.) Exp.	Planes (hkl)	FWHM (deg.)	D (nm)	δ*10^{15} (lines/m^2)	ε*10^{-3}
As-deposited	23.92	111	0.322	26.33	1.44	1.37
	39.24	220				
	46.39	311				
573 K	23.86	111	0.288	29.43	1.15	1.22
	39.27	220				
	46.40	311				
723 K	23.81	111	0.253	33.51	0.89	1.08
	39.26	220				
	46.43	311				

Table 2. Root mean square, average diameter, and roughness average for (CdTe) films at various temperatures.

Annealing Temperature	Root mean square (nm)	Average diameter (nm)	Roughness average (nm)
As-deposited	14.2	71.53	10.8
573 K	16.1	92.22	12.1
723 K	17.1	119.86	13.3

Figure (3a) displays a 2D-AFM image, while **Figure (3b)** displays a comprehensive 3D-AFM image with an outer area of (3μm×3μm). Both reveal topography on CdTe-coated surfaces that were deposited using the spray pyrolysis process at various annealing temperatures. The consistent grain features on the outer layer of the CdTe coating are seen in the 2D AFM micrograph. Additionally, the 3D picture shows a recurrent pattern of valleys and hills that span the whole area under observation. According to the information, the (as-deposited) thin film's root mean square is 14.2 nm and a mean level of roughness of 10.8 nm, to increase the annealing temperature from as-deposited to 723 K, reaching 17.1 nm and 13.3 nm, respectively. This could have happened because films with higher annealing temperatures have better nucleation, coalescence, and continuous growth, all of which increase film quality (27, 28).

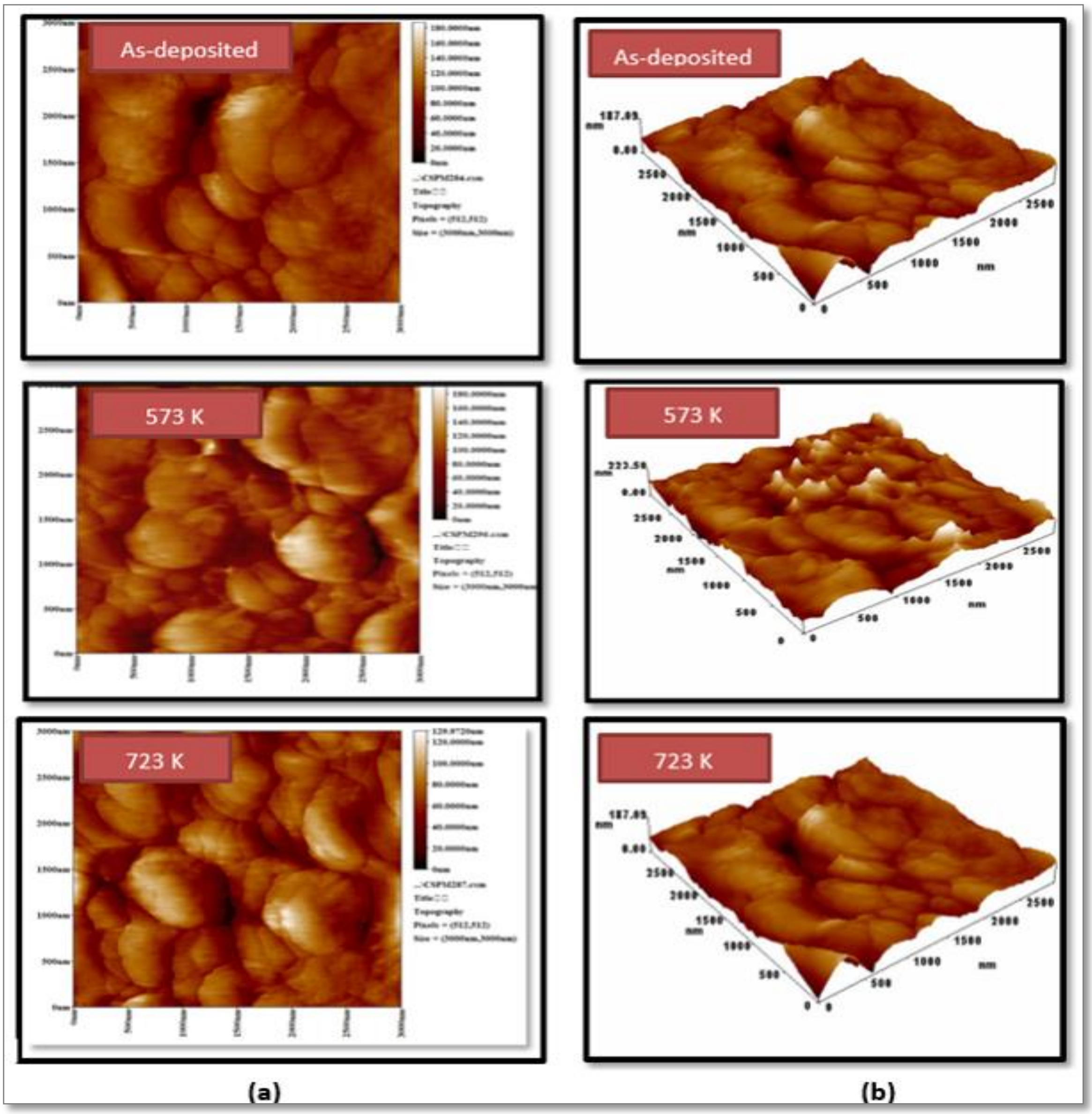

Figure 3. AFM images of thermally annealed and as-deposited on CdTe thin film: (a)AFM-2D (b) AFM -3D.

The AFM data clearly show that this crucial component is the increased surface roughness, which intensifies light scattering. The increased roughness that is created enhances the optical path and increases the likelihood of photon absorption due to full internal reflection (29).

3.2. Optical properties

The CdTe films' transmittance spectrum in the 350–1100 nm spectral region were used to Study their optical characteristics, including the transmittance and absorbance spectra are shown in **Figure (4**) it is discovered that as The temperature at which annealing occurs rises, the optical absorbance of CdTe coating shows a red shift with increasing annealing temperature and also shift towards lower photon energy (with a greater wavelength), which might be explained by the increase in size of grain which was previously supported by XRD and AFM results.

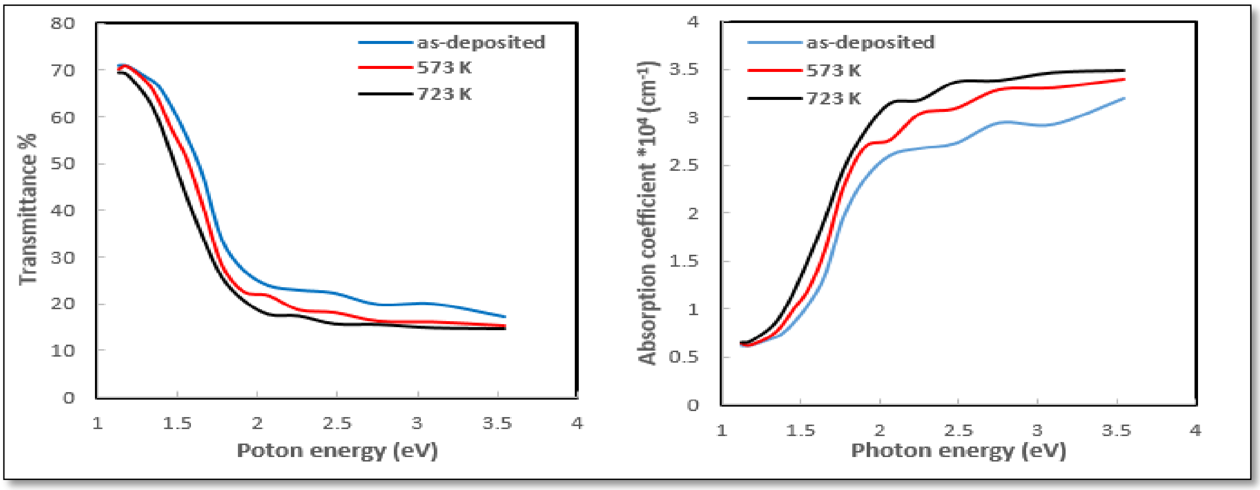

Figure 4. Heat-annealed CdTe thin-film transmittance spectra and absorption coefficient.

Using Tauc's equation, the band gap in optical in CdTe coated films is found (24,29–31).

$$\alpha hv = B(hv - Eg)^r \quad (4)$$

When hʋ denotes incident photon energy, α refers to the absorption coefficient, "B" denotes the energy constant of the material, "Eg" denotes the band gap, and "r" denotes a factual constant. Possessing values for permitted electronic transitions, both allowed direct and indirect, of r = ½ and r = 2.

$$\alpha = \frac{2.303A}{t} \quad (5)$$

When A is the absorbance and t is the film's thickness (32–38). **Figure (5**) displays the band gap's optical energy that is discovered between 1.53 and 1.58 eV and is shown to go down with thermal annealing. This could be because of increased grain size and realignment, as well as a reduction in the number of dislocations and internal strain (39). According to optical band gap analysis, the produced film's dislocation density value is extremely low, indicating that the optical band gap has not increased. The findings are consistent with previously published research (40).

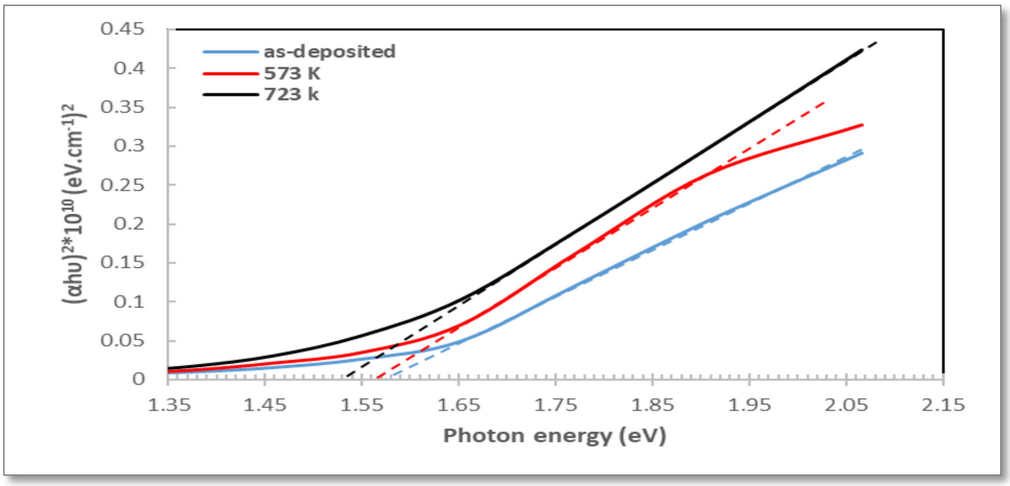

Figure 5. Variation of $(\alpha h\upsilon)^2$ with photon energy ($h\upsilon$) of thermally annealed on CdTe films.

4. Conclusion

This work reports on the improvement of both structural and optical characteristics of CdTe coating annealed. The films crystallize in a cubic form with a favored orientation, according to the structural study (111), as well as being polycrystalline. Changes in the annealing temperature led to an increase in crystallite size from 26.33 to 33.51 nm. The values of microstrain decrease from (1.44 lines/m^2) to (0.89 lines/m^2) and the dislocation density from (1.37 $x10^{-3}$) to (1.08 $x10^{-3}$) with increasing annealing temperatures from the deposited temperature to 723 K, respectively. It is determined that the annealing temperature affects the optical and crystallographic properties. The typical grain size was determined to be between 71.53 and 119.86 nm, and it was seen to rise with annealing. This could have happened because annealing treatment enhances crystallinity. The band gap in optics is between 1.53 and 1.58 eV, and post-annealing treatment is seen to reduce it. The films are homogeneous, consistently packed, flawless, and consistent, according to surface morphological investigations. These findings make it feasible to use the spray pyrolysis approach to create solar cells based on cadmium telluride thin films.

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Conflict of Interest

The authors declare that they have no conflicts of interest.

Funding

We hereby confirm that all the Figures and Tables in the manuscript are ours.

Ethical Clearance

The project was approved by the local ethical committee at the University of Baghdad.

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