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Investigation of Electrical and Optical Properties of CdTe Thin Films Deposited by Thermal Evaporation

Ajay A. Nikam[1],*, Ugalal P. Shinde[2], Mohsin Y. Shaha[1], Mahendra M. Bagul[1]

[1]*Department of Electronics, MVP Samaj's Arts, Commerce and Science College, Dindori, Nashik – 422 202, Maharashtra, India.*
[2]*Sahyadri Shikshan Mandal's M. J. M. Arts, Commerce and Science College, Karanjali, Peth, Nashik – 422 208, Maharashtra, India.*

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ABSTRACT

Preparation and characterization of cadmium telluride (CdTe) thin films via thermal evaporation for capability in optoelectronic applications. After being deposited CdTe on a glass substrate, thin films were electrically and structurally investigated. X-ray diffraction (XRD) confirmed the polycrystalline nature of the films with a preferred orientation along the (111) plane. With characterization of film such as XRD analysis, SEM, etc., the annealing temperature increased, the grain size and crystallinity improved. Hall effect measurements were used to assess electrical characteristics such resistivity, carrier concentration, and mobility. The findings show that optimal thermal evaporation conditions may greatly improve the electrical performance and purity of CdTe films, indicating their potential for effective optical properties.

1. Introduction

Because of its near-optimal bandgap (~1.45 eV) and high absorption coefficient (>10 cm^{-1} in the visible spectrum), cadmium telluride (CdTe) is a well-known semiconductor material that is widely employed in thin-film photovoltaic (PV) technologies [1]. Because of these characteristics, CdTe can absorb the majority of the solar spectrum with just a few microns of material, which makes it appropriate for lightweight and reasonably priced solar cells. CdTe-based solar cells have drawn a lot of interest among commercially available thin-film technologies due to their high efficiency and inexpensive production [2].

The quality and functionality of CdTe thin films are largely dependent on the manufacturing process and post-deposition treatments [3]. CdTe films are frequently deposited using thermal evaporation, a physical vapor deposition (PVD) process, because of its ease of use, capacity to adjust deposition parameters, and appropriateness for creating uniform films across extensive regions. Nevertheless, as-deposited films frequently have surface flaws, high resistivity, and poor crystallinity, all of which have a detrimental effect on their electrical and optical characteristics. As a result, post-deposition annealing is frequently used to improve the films' structural and electrical properties [4]. Prior research has demonstrated that annealing may greatly increase carrier mobility, decrease structural flaws, and improve grain size in CdTe films [5]. These enhancements have a direct impact on the overall efficiency and charge transport characteristics of CdTe solar cells. Optimizing device performance also requires a knowledge of the relationship between electrical qualities like resistivity and carrier concentration and structural factors like crystallite size, preferred orientation, and surface shape. Systematic investigations that assess the impact of annealing temperature on the microstructural and electrical behaviour of films produced via thermal evaporation are still required, despite the advancements in CdTe thin-film research. In order to close this gap, CdTe films will be deposited by thermal evaporation, subjected to controlled annealing treatments, and thoroughly characterized using XRD, SEM, and Hall Effect measurements [6]. The results of this study will help advance thin-film photovoltaic technology and provide more effective solar energy solutions by deepening our understanding of the process-property-performance link in CdTe films.

2. Experimental Methods

2.1 Deposition of Film

A high vacuum thermal evaporation method was used to create thin films of cadmium telluride (CdTe) onto glass substrates that had been properly cleaned. The raw material was 99.99% pure CdTe powder. The substrates were dried under nitrogen flow after being ultrasonically cleaned with acetone, isopropanol, and deionized water to get rid of any impurities. A vacuum chamber with a base pressure of around 2×10^{-3} mbar was used for the deposition. The CdTe material was evaporated using a tungsten boat. A quartz crystal monitor was used to regulate the deposition rate at 1–2 nm/s, and all samples' ultimate film thickness was kept between 550 and 630 nm. To separate the effects of postdeposition annealing, no deliberate substrate heating was used during deposition [7].

2.2 Annealing after Deposition

The as-deposited films were annealed in a muffle furnace with ambient air to examine the impact of thermal treatment. For thirty minutes each, the annealing process was carried out at four different temperatures: 100 °C, 200 °C, 300 °C, and 400 °C. To prevent thermal shock and provide consistent therapy, the heating and cooling procedures were regulated. Characterization of structure Cu Kα radiation ($\lambda = 1.5406$ Å) was used in X-ray diffraction (XRD) at 40 kV and 30 mA to study the films' crystallographic structure. The 2θ range of 20° to 60° was used for the scans. The Debye–Scherrer equation was used to get the average crystallite size (D): $D = 0.9\lambda/\beta\cos\theta$, where λ is the X-ray wavelength, β is the full width at half maximum (FWHM) in radians, and θ is the Bragg diffraction angle.

2.3 Surface Morphology

Scanning electron microscopy (SEM) was used to analyze the films' surface morphology and microstructure. Grain size, surface homogeneity, and the existence of micro-defects or pinholes were all revealed by SEM pictures [8].

2.4 Electrical Characterization

Using a Hall Effect measuring device and the van der Pauw technique, the films' electrical characteristics, such as resistivity, carrier concentration, and Hall mobility, were assessed. Indium solder was used to guarantee ohmic connections. The measurements were conducted in a steady 0.5 T magnetic field at room temperature [9].

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*Corresponding Author:ajay831330@gmail.com(Ajay A. Nikam)

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3. Results and Discussion

3.1 Structural Analysis

The X-ray diffraction (XRD) patterns in Table 1 demonstrate that the CdTe thin films had a cubic zinc blende crystal structure and were polycrystalline in nature. The (111) crystallographic plane, which corresponds to the most dramatic peak at 2θ = 23.8°, shows a high preferred orientation in the growth of the films. Additional diffraction peaks corresponding to the (220) and (311) planes were also present, reflecting the multi-faceted crystalline nature of the deposited films. The calculated crystallite sizes (D), based on the Debye–Scherrer equation, ranged from 17.6 nm to 25.6 nm, with the largest grain size observed for the (111) plane. The progressive increase in crystallite size and the narrowing of full width at half maximum (FWHM) values across the different planes suggest an enhancement in crystalline quality, likely attributable to thermal activation during annealing. These improvements imply reduced lattice imperfections and enhanced atomic ordering within the films. These findings reflect a direct correlation between thermal treatment and enhanced crystallinity, which plays a pivotal role in improving electronic transport mechanisms in CdTe films.

Table 1 Crystallographic details of CdTe films

S. No.	2θ (deg)	Plank (hkl)	FWHM (β) (deg)	Crystallite Size, D(nm)	d-spacing (Å)
1	23.8	(111)	0.3314	25.6	3.73
2	39.2	(220)	0.3934	21.2	2.30
3	46.5	(311)	0.4722	17.6	1.95

3.2 Surface Morphology

Scanning electron microscopy (SEM) revealed significant changes in surface morphology with annealing. At lower annealing temperatures, the surface appeared relatively rough with indistinct grain boundaries. However, as the annealing temperature increased, the grain boundaries became more pronounced, and the overall surface exhibited a denser, pinhole-free structure. Films annealed at 400 °C showed clear grain coalescence and improved surface uniformity, indicative of grain growth and reduced defect density. The transmittance vs wavenumber for CdTe variation shown in Fig. 1 explains these morphological improvements are vital for applications in photovoltaic devices where uniform coverage and minimal defects are crucial for efficient charge transport and reduced recombination losses.

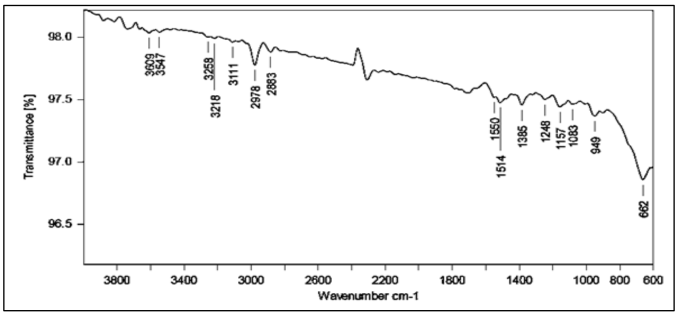

Fig. 1 FTIR (Fourier-Transform Infrared) of spectrum CdTe

3.3 Electrical Properties

Hall Effect measurements demonstrated a substantial enhancement in electrical properties with increasing annealing temperature. The resistivity of the films decreased markedly from 1.9 × 10^6 Ω·cm at 100 °C to 4.8 × 10^5 Ω·cm at 200 °C. This trend was accompanied by a consistent increase in both carrier concentration and mobility. At 200 °C, the carrier concentration reached 3.4 × 10^{14} cm^{-3}, and mobility peaked at 32.6 cm^2/V·s, suggesting significantly improved charge transport characteristics. The observed improvements can be attributed to enhanced crystallinity and larger grain sizes, which facilitate better grain connectivity and fewer trap sites for charge carriers. These characteristics are essential for high-performance optoelectronic devices, including CdTe-based solar cells [10].

3.4 Discussion

The crucial significance of thermal treatment in improving material characteristics for photovoltaic applications was demonstrated by the structural and electrical study of CdTe thin films deposited via thermal evaporation, which showed notable modifications as a result of post-deposition annealing.

3.4.1 Structural Improvements

The polycrystalline character of the CdTe films with a preferential orientation along the (111) plane was confirmed by X-ray diffraction (XRD) analysis, which is in keeping with the normal development habit of CdTe crystals. Full width at half maximum (FWHM) narrowed and peak intensity systematically increased as the annealing temperature rose from 100 °C to 400 °C, suggesting better crystallinity. Because of the decrease in internal stress and grain boundary flaws during annealing, the predicted crystallite size increased with temperature. Atomic ordering inside the lattice is improved and dislocations are decreased by this grain coalescence and rearrangement. Charge carrier paths are directly impacted by the preferred orientation and crystallinity since a well-aligned grain structure allows for more effective transport with fewer scattering occurrences. These findings are consistent with other research that indicates post-deposition annealing at moderate to high temperatures encourages recrystallization and produces more defect-free films appropriate for solar cell applications.

3.4.2 Surface Morphology Evolution

The films' surface morphology significantly improved after annealing, according to scanning electron microscopy (SEM). The films showed a comparatively granular and inhomogeneous structure with discernible micro voids at lower temperatures (100–200 °C). Nevertheless, the films grew more compact, with smoother surfaces and clearly defined grain boundaries, at higher temperatures (300–400 °C). Fig. 2 shows wavelengths for 1.5406 / 1.54433, while Figs. 3 and 4 shows SEM image of Pure CdTe with 0.5µm and 5.0µm and 10% Zn doped CdTe with 5.0µm and 1.0µm. Increased grain growth and film densification, which are advantageous for lowering surface recombination losses in solar cell structures, are suggested by this morphological development. Better adhesion and interface formation with other layers in a conventional thin-film solar cell, such the CdS buffer layer or a transparent conductive oxide, are also implied by such increases in film uniformity.

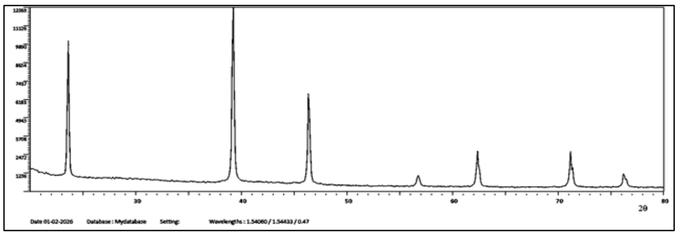

Fig. 2 XRD of Pure CdTe

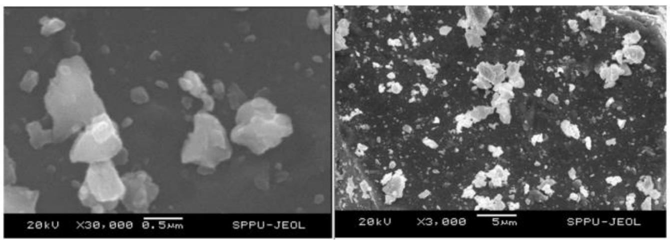

Fig. 3 SEM of Pure CdTe with 0.5 µm and 5.0 µm

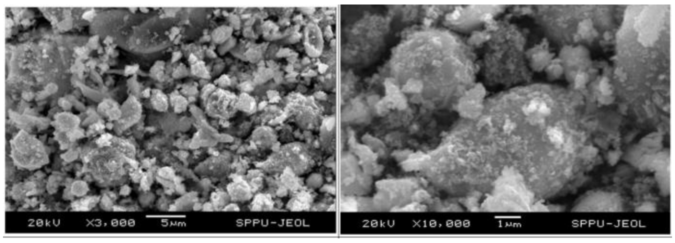

Fig. 4 SEM of 10% Zn doped CdTe with 5.0 µm and 1.0 µm

3.4.3 Charge Transport and Electrical Properties

Additional proof of annealing-induced amplification came from electrical tests. Resistivity dramatically dropped as the annealing temperature rose, whereas carrier concentration and mobility rose. The passivation of defects like vacancies and interstitials, which serve as charge carrier trap centres, can account for this behaviour. Improved crystallinity and decreased grain boundary resistance are probably the causes of the increased mobility, which implies that charge carriers come into contact with fewer scattering locations. The films showed the best

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charge transport characteristics at 400 °C, with the lowest resistance and maximum mobility. These features are crucial for photovoltaic systems because they make it possible for photogenerated carriers to be efficiently collected and transferred, increasing the power conversion efficiency. Notably, the electrical behaviour that has been observed aligns with the previously mentioned structural enhancements. The relationship between mobility and grain size highlights how crucial it is to produce big, homogeneous grains in order to decrease recombination sites and lengthen carrier lifespan.

3.4.4 Consequences for Photovoltaic Uses

The results of this work demonstrate that thermal evaporation may produce CdTe thin films with desired structural and electrical characteristics for solar cell construction when combined with appropriate annealing processes. Thermal evaporation is still a viable, affordable option, especially for research and prototyping, even though methods like close-spaced sublimation (CSS) and metal-organic chemical vapor deposition (MOCVD) are more frequently employed for commercial CdTe solar cells. The possibility of employing this technique in scalable PV systems is highlighted by the improvement of material characteristics by a rather straightforward post-treatment. To assess overall cell performance and stability, however, more research into optical characteristics, junction creation, and comprehensive device integration is required.

4. Conclusion

The structural, morphological, and electrical characteristics of cadmium telluride (CdTe) thin films produced by thermal evaporation and exposed to post-deposition annealing at different temperatures were methodically examined in this work. The findings unequivocally show that annealing greatly improves the quality of CdTe thin films. With increasing annealing temperatures, XRD analysis showed enhanced crystallinity and larger grains, especially at 400 °C, when the films showed strong (111) orientation and fewer lattice defects. These conclusions were corroborated by SEM images, which demonstrated improved grain development and surface homogeneity. Electrical experiments showed significant increases in carrier concentration and mobility as well as a significant reduction in resistivity, particularly for films annealed at higher temperatures. These results validate that a crucial process parameter for maximizing the performance of thermally evaporated CdTe thin films is post-deposition annealing. These films are good options for use in thin-film photovoltaic systems because to the improvements in crystallinity, surface morphology, and electrical properties. To further confirm that these films are suitable for high-efficiency solar cells, further research may involve optical analysis, device-level integration, and long-term stability testing. The study's findings advance the area of thin-film photovoltaics and aid in the creation of high-performing, reasonably priced CdTe-based solar energy solutions.

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