Performance analysis of CdS-based thin films in photovoltaic applications

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Cadmium sulfide (CdS) thin films are extensively utilized as a window layer in photovoltaic (PV) devices due to their high transmittance, suitable bandgap, and favorable electrical properties. This work presents a comprehensive performance analysis of CdS based thin films in PV applications, examining key factors such as optical, electrical, and structural properties. The bandgap (approximately 2.42 eV) allows effective photon transmission, reducing energy losses. Critical performance metrics, including film thickness, grain size, crystallinity, and interface quality with the absorber layer, are optimized to enhance charge separation and minimize recombination losses. The study highlights the balance between thin-film transparency and thickness to maximize photon absorption while ensuring film durability and stability in environmental conditions. The findings underscore the potential of CdS thin films to improve PV cell efficiency, offering insights into achieving higher fill factor (FF), short-circuit current (Jsc) and open-circuit voltage (Voc) in CdS-based PV devices.

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1. Introduction

Now a days, solar energy is crucial for power generation because it is a renewable, environmentally friendly resource that reduces reliance on fossil fuels. It offers long-term cost savings and energy independence while helping to combat climate change. A solar cell is a key component in a solar energy system, converting sunlight directly into electrical energy through the photovoltaic effect. It serves as the primary unit for capturing and transforming solar energy into usable electricity for various applications. In 2009, global production of PV cells reached about 12.3 GW [1]. So various types of solar cells have been developed for more energy production using thin-film technology [2, 3], silicon [4] and organic materials [5-7]. The U.S. Department of Energy states that large-scale solar energy production will become economically viable once the cost is reduced to $0.33 per watt-peak (Wp).

Thus, Cadmium Telluride (CdTe) is a key material in thin film solar cells due to its high efficiency, optimal bandgap and excellent light absorption properties. It enables cost effective and lightweight solar panels with a simpler manufacturing process compared to silicon based technologies. The theoretical efficiency of CdTe thin-film solar cells is estimated to be around 28–30%. This efficiency is determined by the material's optimal bandgap of ~1.45 eV and its excellent light absorption properties. [8, 9]. But its commercial efficiencies typically range between 15-18%, which is lower than high-efficiency silicon cells.

To overcome this drawback, CdS is used in conjunction with CdTe in solar cells as a transparent window layer due to its wide bandgap (~2.42 eV), allowing sunlight to pass to the CdTe absorber. It provides good lattice matching with CdTe, reducing defects and improving efficiency. CdS also facilitates high-quality p-n junction formation and is easy to deposit using standard techniques, making it an ideal choice for optimizing CdTe solar cell performance. [10].

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Recently, CdS thin films are fabricated using a variety of techniques [11,12], including Sputtering, chemical bath deposition (CBD) [13,14], Electro deposition, sol-gel [16] and some other methods [15]. However, these techniques often require expensive equipment, a controlled environment, and strict operational conditions. In addition to these established methods, emerging techniques like successive ionic layer adsorption and reaction (SILAR) etc., have been introduced for synthesizing CdS nanoparticles [17,18].

Apart from all these methodologies, Spray pyrolysis is a cost-effective, scalable technique suitable for large-area deposition of thin films. It offers precise control over film thickness and produces homogeneous coatings. The method works at relatively low temperatures, making it ideal for heat-sensitive substrates. It is versatile, capable of depositing a wide range of materials.

In this study, CdS thin films were synthesized using a Spray pyrolysis method. This approach is easily scalable for large-area deposition of CdS thin films. The synthesized films were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), Raman spectroscopy, and Fourier-transform infrared (FTIR) spectroscopy to examine their phases, structures and surface morphology, highlighting their potential for CdS solar cell applications.

2. Experimental details

2.1. Spray pyrolysis method

It is a versatile and cost effective technique used for fabricating thin films. For the preparation of CdS, solutions containing cadmium precursors and thiourea., were prepared in 20 ml of double-distilled water. The thiourea reacts with cadmium ions during deposition and forms cadmium sulfide (CdS) thin films on the heated substrate at 400°C. This method atomizes this precursor solution into fine droplets that are sprayed onto the heated substrate. The high temperature of the substrate causes thermal decomposition of the precursors, leading to the formation of CdS films. Thiourea is chosen here as sulfur source for CdS thin films because it is cost effective and readily available.

3. Characterization techniques

The characteristics of the prepared thin films were analyzed using XRD patterns obtained from a Rigaku MiniFlex desktop diffractometer at a wavelength of 1.5406 Å. SEM was utilized to analyze the morphology and determine the grain size of the films. The optical properties were investigated using a UV-VIS spectrophotometer (JASCO V-670), covering the wavelength range of 300–1000 nm. Luminescence characteristics were examined using a Fluoromax-4 spectrophotometer.

4. Structural studies

4.1. XRD analysis

XRD analysis revealed peaks at 26.5°, 44°, and 52°, corresponding to the (111), (220), and (311) crystallographic planes, respectively, as illustrated in Figure 1.. These peaks confirms the formation of thin films. The diffraction patterns confirm a cubic nature of CdS by highlighting its polycrystalline nature.

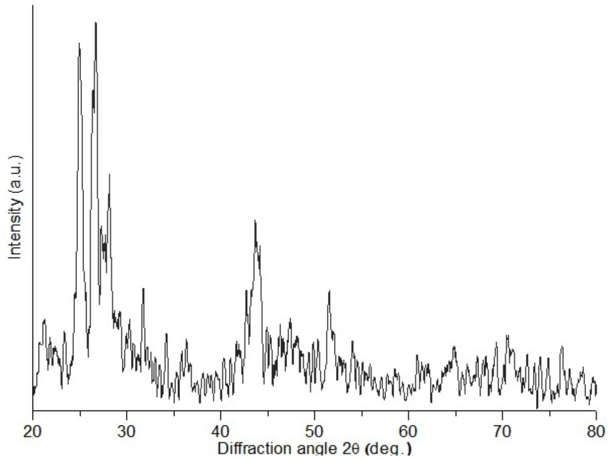

Fig. 1. XRD analysis of the CdS-based thin films

Table 1. Structural characteristics - CdS thin films.

2θ (degree)	Crystallite size D (nm)	Dislocation Density (δ) ($x10^{16}$ lines/m^2)	Stacking fault (Å)
26.50	7.18	1.9397	0.010344
43.82	6.23	2.5803	0.009577
51.74	3.84	6.7724	0.014569

From the above table, the δ is found to be inversely proportional to D. A low dislocation density indicates that spray pyrolysis is an effective technique for depositing high-quality polycrystalline CdS thin films.

4.2. FTIR study

The bonding and structural properties of the synthesized CdS films were analyzed using FTIR spectroscopy, with the corresponding spectra presented in Figure 2.

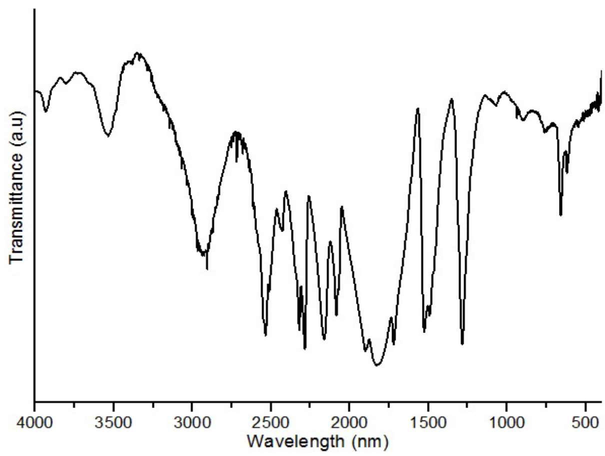

Fig. 2. FTIR characteristics of the CdS-based thin films

The Cd $3d_5/_2$ and Cd $3d_3/_2$ peaks are the most prominent, typically appearing around 404–413 eV. These peaks confirm the presence of cadmium in the CdS thin film. Symmetric and sharp peaks indicate that cadmium is in a well-defined chemical environment, within the CdS matrix.

4.3. XPS analysis

The XPS spectrum (Figure 3) can confirm the presence of cadmium sulfide (CdS) by identifying characteristic peaks. Key peaks to look for are the Cd $3d_5/_2$ at 405 eV and Cd $3d_3/_2$ at ~412 eV, which indicate the presence of Cd^{2+}, and the S $2p_3/_2$ at ~161.5–162 eV and S $2p_1/_2$ at ~163 eV, corresponding to S^{2-}. These peaks are signatures of CdS and confirm its presence.

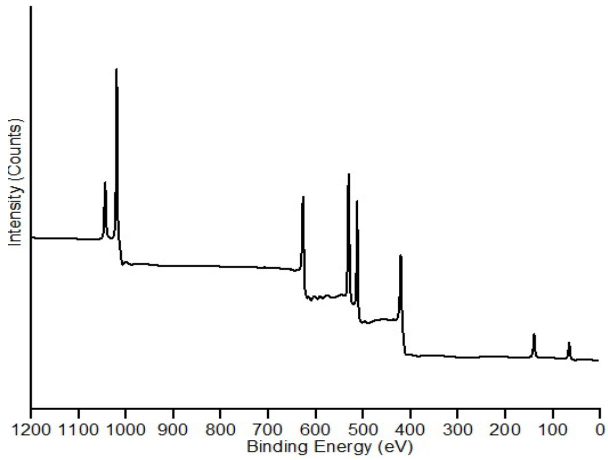

Fig. 3. XPS analysis of the CdS-based thin films

5. Optical properties of CdS

5.1. Morphological and elemental analysis

Morphological analysis of CdS involves studying the surface structure, texture and grain distribution of the material. SEM is typically employed for this purpose, providing high-resolution images to observe features like grain size, uniformity and compactness. This analysis helps in understanding the film's growth mechanism, surface defects, and overall quality, which are crucial for optimizing its performance in applications.

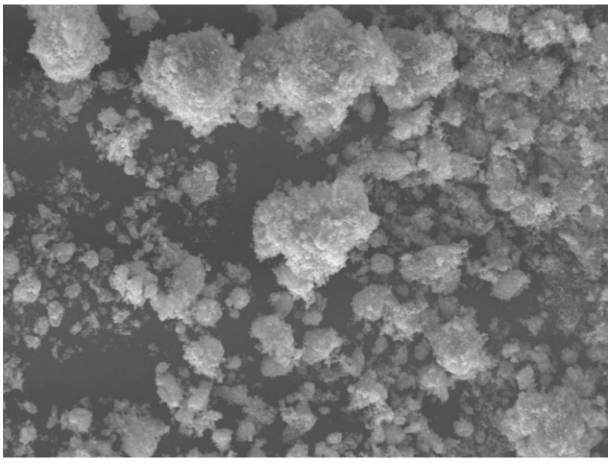

Fig. 4. SEM analysis of the CdS-based thin films

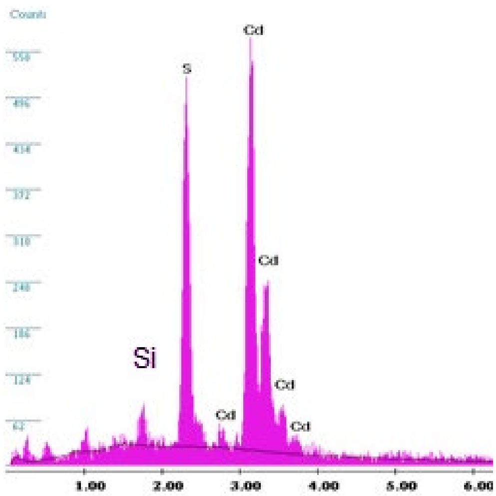

Fig. 5. EDX of the CdS-based thin films

This SEM image represented in figure 4 reveals the surface morphology of the CdS thin film, showing an agglomeration of particles with a rough, clustered structure. The clustered, agglomerated particles in the CdS thin film suggest a high degree of surface roughness. In PV applications, a rough surface can increase light scattering and enhance light absorption within the absorber layer below as it is used as a window layer. This can improve the overall efficiency by trapping more light within the cell. The rough morphology may suggest some porosity in the film. However, the size of porosity is small in this case, it can reduces the reflectance and improves the adhesion to the substrate. Thus, good adhesion ensures the durability of the cell during thermal cycling and under environmental stress.

The EDX spectrum (figure 5) shows clear peaks for cadmium (Cd) and sulfur (S), confirming the successful synthesis of CdS, which is essential for PV applications. In this, the Cd ratio appears to be balanced, suggesting optimal stoichiometry for efficient charge generation. A small silicon (Si) peak indicates the presence of the substrate, typical in thin-film PV devices. No significant impurities are observed, indicating relatively pure CdS. Overall, the film seems promising for use in CdTe-based solar cells.

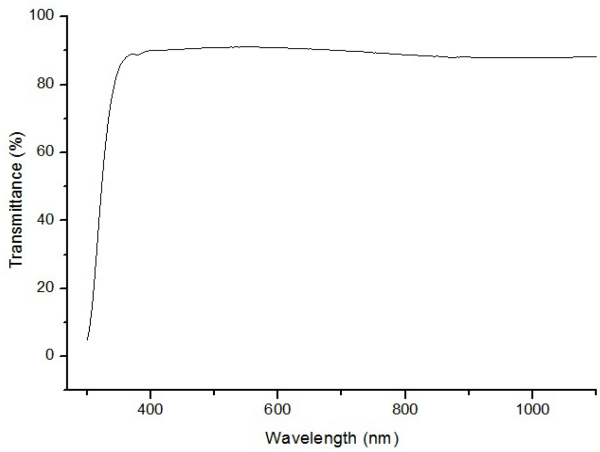

Fig. 6. Transmittance analysis of the CdS-based thin films

The transmittance spectrum of CdS thin films (figure 6) shows a sharp increase in transmittance above approximately 400 nm, reaching values above 80%, indicating that the film is highly transparent in the visible region. The sharp rise suggests a well-defined bandgap, characteristic of CdS, where light absorption significantly drops after the onset of absorption around 400 nm. The high transmittance in the visible range is advantageous for PV, as it allows more light to pass through to the underlying active layer, enhancing the efficiency of the solar cells. The low transmittance in the UV region indicates absorption due to the material's bandgap.

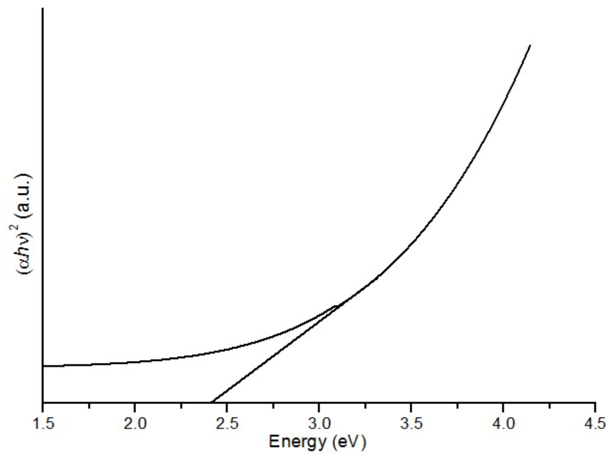

Fig. 7. Optical bandgap of the CdS-based thin films

The intersection points on the x-axis in figure 7 gives the band gap energy, Eg of the CdS film. This value represents the minimum photon energy required for electronic transitions from the valence to the conduction band, indicating the optical band gap of the material. In this plot, it appears that the linear portion extends to approximately 2.4–2.5 eV on the energy axis. This bandgap of 2.4 eV makes CdS highly transparent to visible and near-infrared light, allowing most of the solar spectrum to reach the underlying absorber layer, thus enhancing photocurrent. Additionally, the higher bandgap reduces recombination losses by blocking minority carriers, leading to an improved open-circuit voltage (Voc) in solar cells. This makes it an excellent candidate for use as a window layer in solar cells.

Thus, it is proven that CdS films have been shown to be chemically and thermally stable, which is essential for the long-term durability of solar cells.

6. Performance metrics

The performance of CdS-based thin-film solar cells is typically evaluated using the following key metrics, Power Conversion Efficiency (PCE), Voc, Jsc, FF and Stability and Durability.

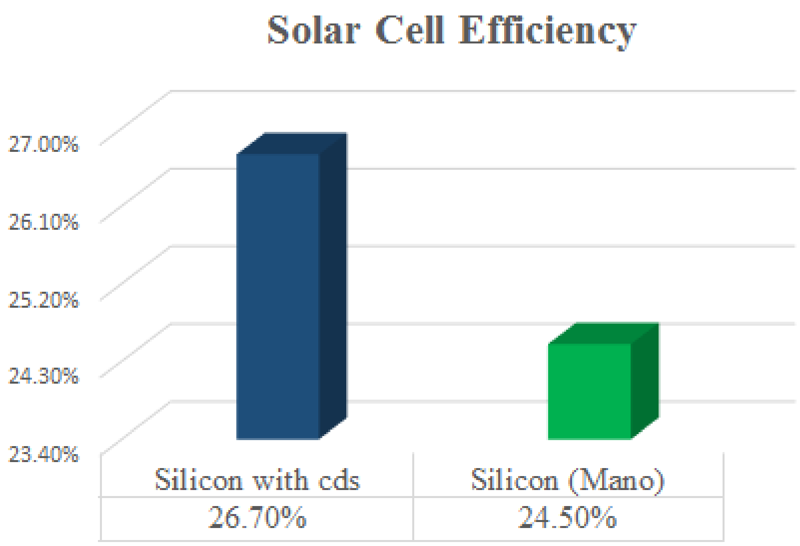

Fig. 8. PCE comparison of the silicon based solar cells

Figure 8 compares the PCEs of silicon cells and silicon based solar cells incorporating CdS as a window layer. This highlights the slight efficiency reduction typically observed when using silicon, likely due to optical losses or interface recombination [19-21].

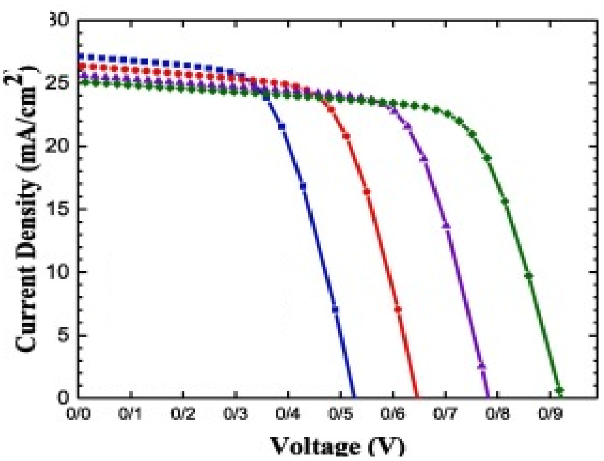

Fig. 9. Current density Vs voltage of the silicon based solar cells

The figure 9 provides critical insights into the J−V characteristics of photovoltaic devices. The variation in Voc suggests the efficiency of this application can be improved material and structural modifications.

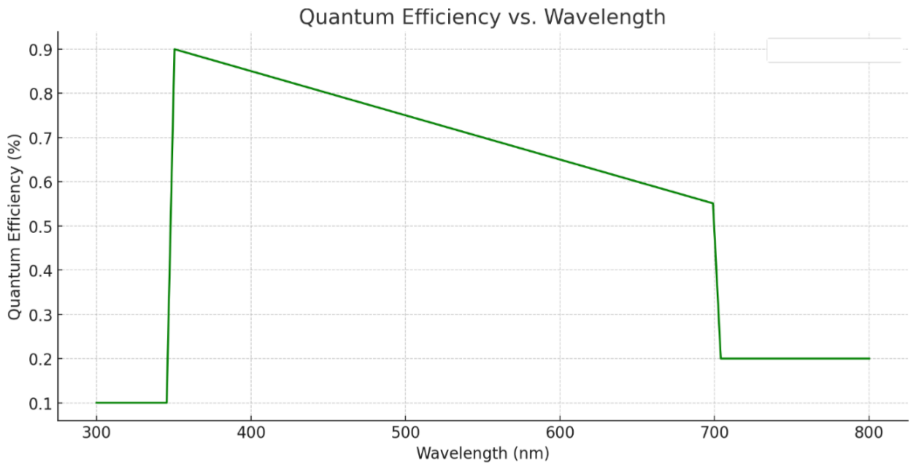

Fig. 10. Quantum Efficiency of the silicon based solar cells

Figure 10 depicts the Quantum Efficiency (QE) of a material as a function of wavelength, with a sharp rise in efficiency between 300-400 nm (UV region), indicating high absorption in the UV range. After 400 nm, QE decreases, with a steep drop after 700 nm, showing low efficiency in the visible and near-infrared (NIR) spectrum. This behaviour is typical of CdS-based thin films, which absorb well in the UV but have limited effectiveness in the visible and NIR ranges, making them ideal as a window layer in solar cells.

7. Conclusion

CdS thin films were deposited on glass substrates using the spray pyrolysis technique. The films' structural and optical properties were analysed. XRD results confirmed a cubic phase structure of the CdS thin films, while SEM images revealed that the samples superior uniformity and minimal defects. The optical band gap values were measured within the range of 2.16-2.43 eV. The findings underscore the effectiveness of CdS thin films as a window layer in PV applications, with significant potential for enhancing cell performance.

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