

EFFECTS OF THERMAL TREATMENTS ON FUNCTIONAL GROUPS AND PHOTOMETRIC MEASUREMENTS OF THERMALLY EVAPORATED CdS FILMS FOR PV APPLICATIONS

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ABSTRACT

This paper investigated the effects of thermal treatments on the functional groups and optical properties of thermally evaporated CdS films for photovoltaic applications. The synthesized CdS nano-particles were evaporated from molybdenum boat and deposited on clean glass substrates as thin films form. 100 nm CdS films were ensured on glass substrates via thermal evaporation in a residual pressure of 10-5 Torr and substrates at room temperature. The obtained CdS films were annealed at 400 and 500°C respectively. All samples were characterized using UV-VIS Spectrophotometer. The absorbances of the films were calculated from the transmittance data using Beer's Lambert law. ALPHA II FTIR Spectrometer was employed to investigate the vibrations of the functional groups of CdS films at the respective annealing temperatures under study. Powder X-Ray Diffractometer (PXRD) was used to confirm the phase of the CdS prior to and after the deposition. The results revealed maximum transmittances of about 90 % for all samples at the CdS prior to and after the deposition. The results revealed maximum transmittances of about 90 % for all samples at 656, 657 and 646 nm wavelengths respectively and varied at other wavelengths. The vibrations of the functional groups of CdS films were not perturbed by the annealing temperatures under study and the energy band gaps of 2.42, 2.4 and 2.9 eV were estimated for the as grown, 400 and 500 °C CdS films respectively. Based on the obtained results, 100 nm CdS film deposited via thermal evaporation and annealed at 400 °C is hereby encouraged for the development of CdS/CdTe polycrystalline thin film solar cells.

Keywords: CdS, Glass substrate, thermal evaporation, annealing temperature, Energy band gap.

INTRODUCTION

In CdS/CdTe solar cell research and development programme, thermal treatment has been found to be a key step for drastic improvement of the solar to electric conversion efficiency (Dharmadasa, 2014, Romeo *et al.*, 1999 and Mendoza *et al.*, 2005). Cadmium Sulphide (CdS), belonging to the II-VI group, is an *n*-type direct band gap semiconductor ($E_g = 2.42$ eV) (Awodugba *et al.*, 2014, Abdulmakarim *et al.*, 2014, Rinu *et al.*, 2015, Arunraja *et al.*, 2014 and Zahid *et al.*, 2011). It is studied extensively because of its band gap, higher absorption coefficient, reasonable conversion efficiency, good stability and low cost (Elmas *et al.*, 2012).

The low cost and large area thin film formulation of CdS is necessary for technological application as window material for CdS/CdTe solar cells, light emitting diodes for flat panel displays and transistors for electronic switches, optical filters, photo

detectors, gas sensors and piezoelectric transducers, laser materials, optical wave guides, and nonlinear integrated optical devices (Igbal, 2013, Shah *et al.*, 2014, Selma *et al.*, 2009, Djelloul *et al.*, 2016 and Hasnat and Podder, 2012).

Awareness of some physical properties such as optical, morphological and structural characteristics of CdS films is very important in many scientific and technological applications in the field of optoelectronic devices, especially photovoltaic solar cells (Elmas *et al.*, 2012 and Jun *et al.*, 1998). Also, the effect of thermal treatments on CdS films have also been established by several researchers but attentions are not much focused on the vibrations of the functional groups of the annealed CdS films particularly at the temperature suitable for thin film solar cell development. Also, the growth technique and the required thickness suitable for window layer of CdS/CdTe solar cell are still open for discussion. Hence, in this work, we reported the influence of thermal treatments on vibrations of

functional groups and optical properties of 100 nm CdS thin films deposited via thermal evaporation technique for photovoltaic applications.

MATERIALS AND METHOD

The synthesized CdS nano particles were employed for the deposition of 100 nm CdS films on glass substrates via thermal evaporation and characterized using ARL X'TRA Powder X-Ray Diffractometer (PXRD) to confirm the phase of the nano particles prior to and after the deposition. CdS nano particles were evaporated from molybdenum boat and deposited on clean glass substrates as thin films form in a residual pressure of 10^{-5} Torr. The substrates temperature was kept fixed at room temperature and the fabricated films were annealed at 400 and 500 °C respectively. The as-grown and the annealed CdS films were characterized via AvaLight-DH-S-BAL UV-VIS-NIR Spectrophotometer to measure the percentage reflectance and transmittance of the films under study. The absorbances of the films were measured from transmittance data using Beer's Lambert law. The absorption co-efficient and optical band gaps were also determined. The ALPHA II Fourier Transform Infrared

(FTIR) Spectrometer was used to investigate the vibrations of the functional groups of CdS films at respective annealing temperatures under study. The absorption coefficient (α) is calculated from transmittance data using eqn 1.

$$\alpha = \frac{2.303 (2 - \log_{10} \% T)}{t} \quad (1)$$

Where T is the transmittance and t is the thickness of the film.

The absorption coefficient (α) can be written as a function of incident photon energy ($h\nu$). The electronic transitions between the valence and conduction band is given by (Khusayfan and El-Nahass, 2013).

$$\alpha h\nu = A(h\nu - E_g)^P \quad (2)$$

Where A is a constant. E_g is the optical band gap energy and P has discrete values like $\frac{1}{2}$, $\frac{3}{2}$, 2 or more depending on whether the transition is direct or indirect and allowed or forbidden. For the direct and allowed case $P = \frac{1}{2}$, and for forbidden case, P is $\frac{3}{2}$ or more.

RESULTS AND DISCUSSION

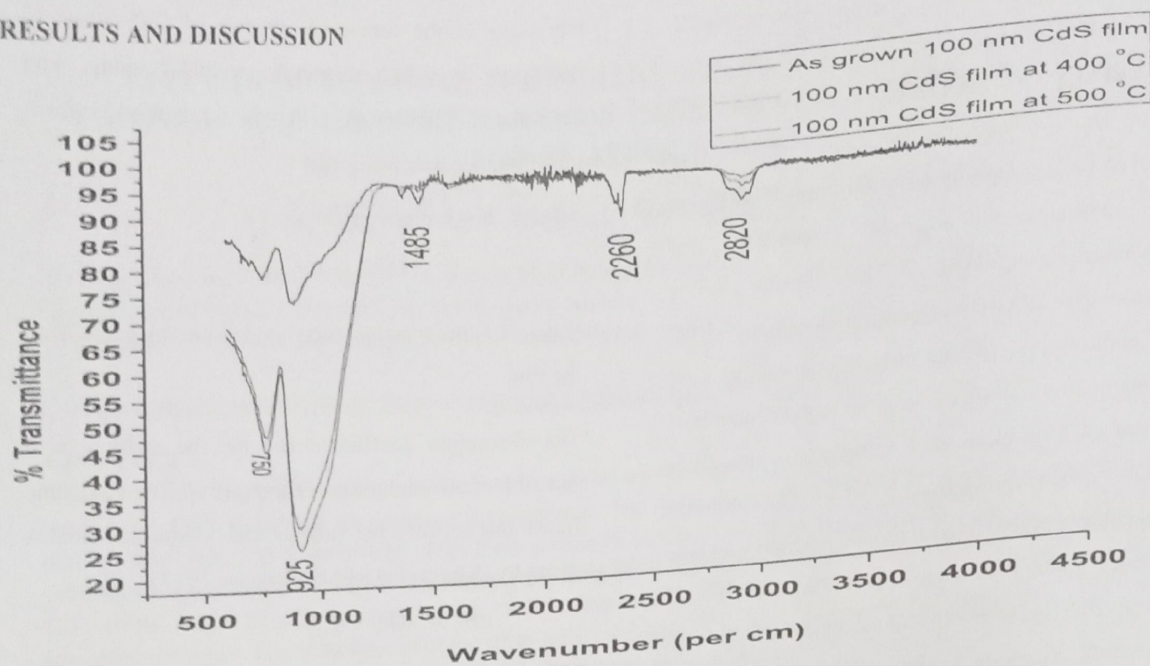


Figure 1: Fourier Transform Infrared (FTIR) spectra of 100 nm CdS films at different temperatures

Figure 1 shows the FTIR spectra of 100 nm CdS films annealed at different temperatures. The FTIR spectra of 100 nm CdS films showed different absorptions bands at different wave number. The percentage transmittance against the wave number (cm^{-1}) varies for each film and each absorption band related to different chemical bonds of the CdS. These bands are listed in Table 1. The transmittances of the CdS films were affected by the

annealing temperatures (as grown, 400 and 500 °C) without the observed changes in the vibrations of the functional group of the CdS. The characteristic absorption frequencies includes Methylene (CH_2)_n rocking, Methylene C-H bend, Medial alkyne (di-substituted), Methoxy, C-H stretch and Cyclohexane ring vibrations.

Table 1: Group frequency wave number and origin related to absorption band of 100 nm CdS films

Origin	Group frequency wave number (cm^{-1})	Assignment
C-H	750	Methylene (CH_2) _n rocking
C-H	925	Cyclohexane ring vibrations
C-H	1485	Methylene C-H bend
C=C	2260	Medial alkyne (di-substituted)
C-H	2820	Methoxy, C-H stretch

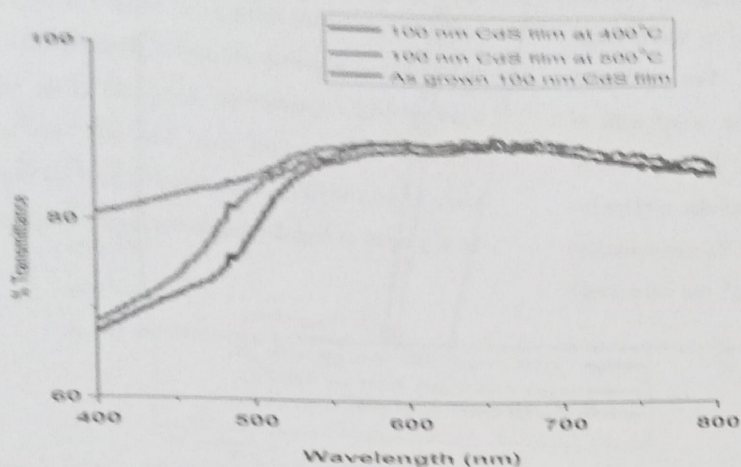


Figure 2: % Transmittances of 100 nm CdS thin films annealed at different temperatures

The percentage transmittance characteristics of CdS films are shown in figure 2 as function of wavelengths. The percentage transmittances of as-grown, 400 and 500 °C annealed 100 nm CdS films were compared. The percentage optical transmittances of the films increased from very low values to maximum values as the wavelength increases in the visible to near infrared region of the solar spectrum. This behavior may be attributed to difference energies at respective wavelength and temperature annealing effect. The

maximum optical transmittances of 100 nm CdS films for as-grown, 400 and 500 °C annealed films were about 90 % at 656, 657 and 646 nm wavelength respectively. The observed transmittances for the films were comparable around 550 nm wavelengths and above owing to the thermal evaporation technique of deposition employed with exclusion of impurities. The thermal treatment effects were more pronounced at around 400 to 550 nm wavelength in the visible region of the solar spectrum.

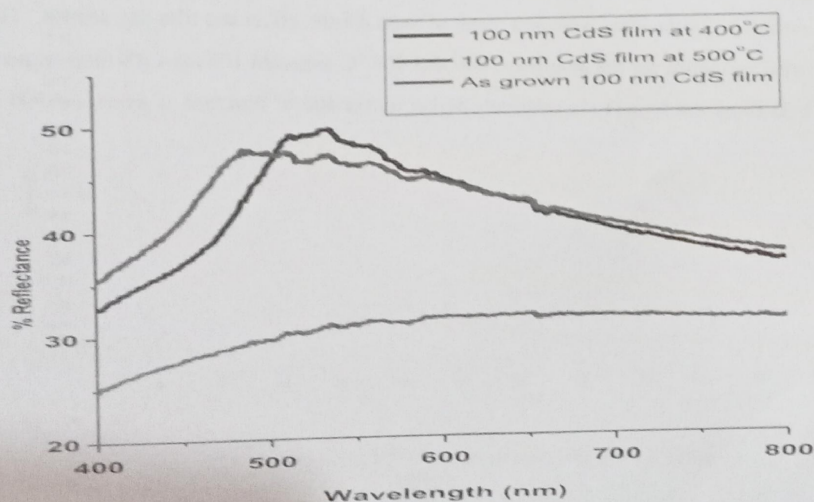


Figure 3: % Reflectance of CdS films annealed at different temperatures

The percentage reflectance of as-grown, 400 and 500 °C annealed CdS films were compared in figure

3. The magnitude of reflectance spectra of CdS thin films varied with annealing temperatures and

wavelengths. Several oscillations observed on the reflectance spectra may be attributed to interferences amidst multiple reflected waves. The oscillation periods of the films changes as the wavelength of electromagnetic wave increases. This behaviour depends strongly on the wavelength of electromagnetic spectra. Highest reflectance of 47.76 % was estimated at 488 nm wavelength, 49.4 % at 535 nm wavelength

and 31.4 % at 602 nm wavelength for the as-grown, 400 and 500 °C annealed 100 nm CdS films. The percentage reflectance of as grown and 400 °C annealed CdS films were relatively symmetrical compared to the 500 °C annealed 100 nm CdS film. The non -interference phenomenon of 500 °C annealed 100 nm CdS film may be as a result of film degradation at higher temperatures.

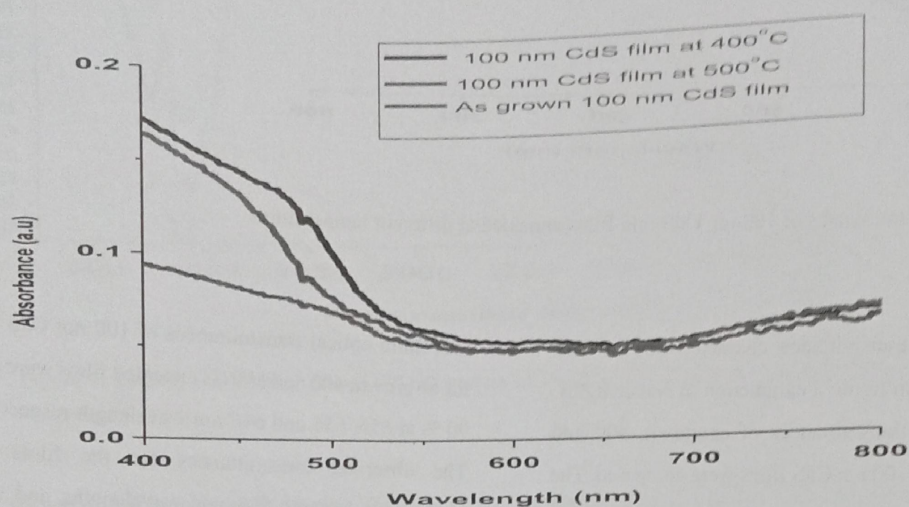


Figure 4: Absorbance of 100 nm CdS films annealed at different temperatures

It was observed from the absorbance spectra in figure 4 that the absorbances of the films decreased with increasing wavelength from 400 to about 650 nm wavelengths and begins to increase to near infrared region of the solar spectrum. The energy of the photons at some respective wavelengths from 400 to about 650 nm wavelength was higher than the energy band gap of CdS and this was responsible for the relatively higher absorptions at shorter wavelength. Different absorbances estimated for the films were as a result of mass density effect and film degradation. The values of 0.165, 0.17 and 0.092 were estimated for the as-grown, 400 and 500 °C annealed 100 nm CdS films respectively. The absorbance of 100 nm CdS films was found to be relatively higher for the 400 °C film than as grown and 500 °C annealed films.

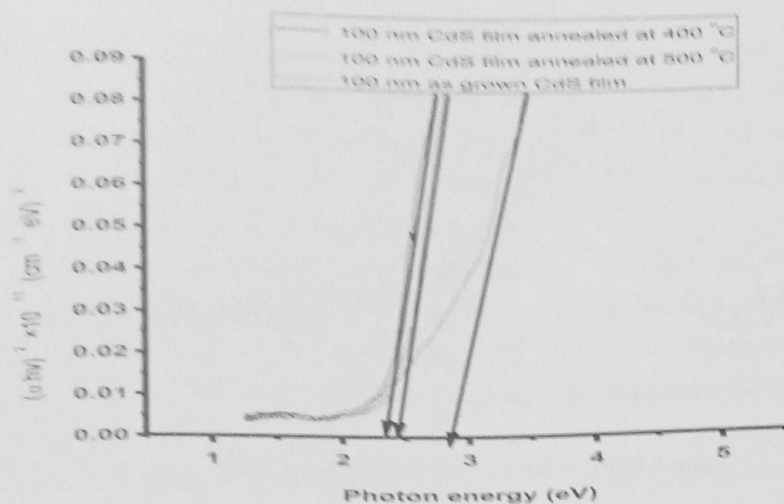


Figure 5: Energy band gaps of 100 nm CdS films annealed at different temperatures

Figure 5 shows the energy band gaps of 100 nm CdS films annealed at different temperatures. The optical band gap energies were determined by extrapolating the straight line of the Tauc plot for zero absorption coefficients ($\alpha = 0$). The optical energy band gap varies with annealing temperatures due to thermal effect. The optical energy band gaps of 2.42 and 2.4 eV were estimated for the as-grown and 400 °C annealed 100 nm CdS films. The decrease in the optical energy band gaps are in accordance with the reported work of (Pantoja, 2013 and Hasnat and Podder, 2012). At annealing

temperature of 500 °C, 2.9 eV was estimated for the 100 nm CdS film. The increase in the energy gap may be due to film degradation and polycrystalline phase change of CdS at annealing temperatures above 400 °C. The parameters and process that affected the band gaps are grain size, strain, dislocation density, crystalline phase change from cubic to hexagonal, sulfur and cadmium evaporation that affect films stoichiometry, oxidation and degradation of the film at annealing temperatures above 400 °C.

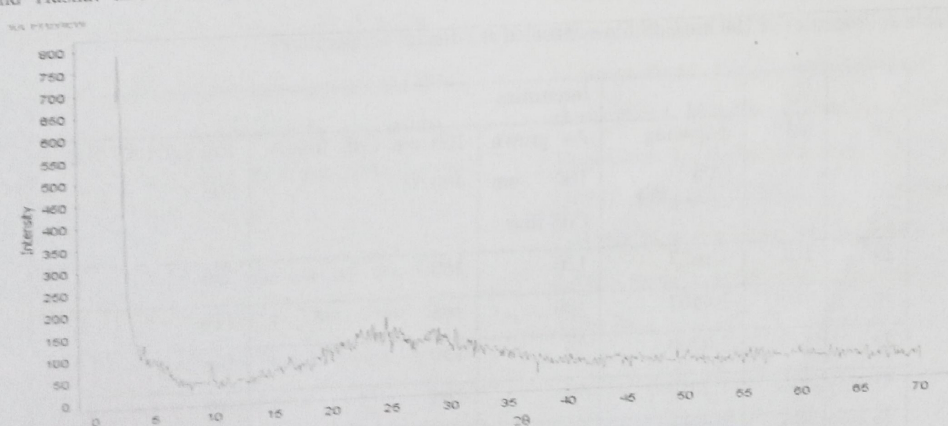


Figure 6: PXRD of as grown 100 nm CdS film

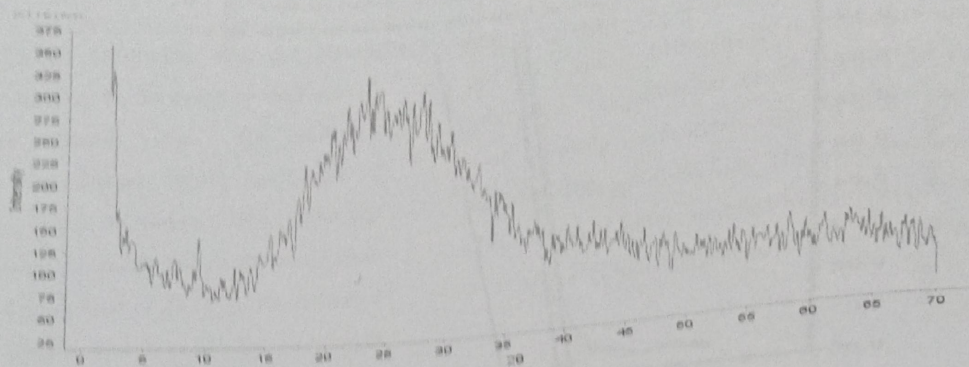


Figure 7: PXRD of 100 nm CdS film annealed at 400 °C

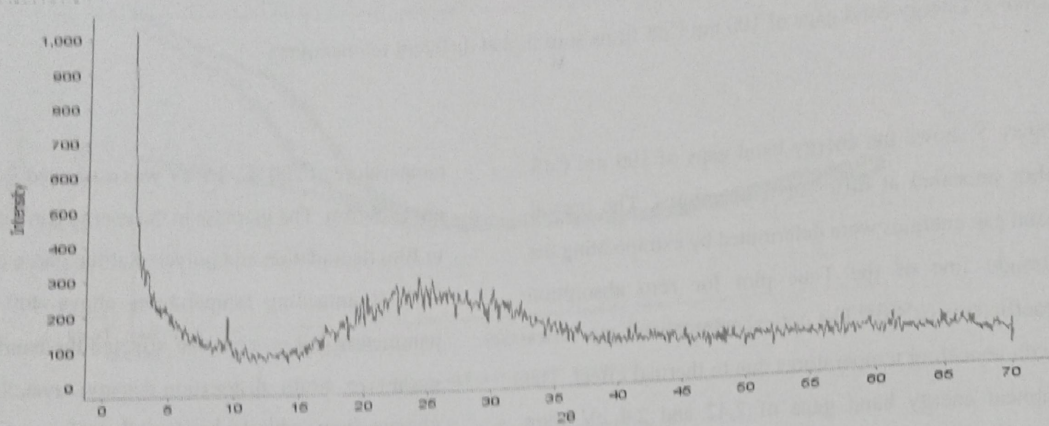


Figure 8: PXRD of 100 nm CdS film annealed at 500 °C

Table 1 below showed the diffraction Bragg's angle, Miller indices, inters planar spacing and the intensities of 100 nm CdS films at different temperatures.

Table 2: Properties of 100 nm CdS films annealed at different temperatures

2θ	hkl	d-spacing (Å)	Intensities		
			As grown 100 nm CdS film	100 nm CdS film at 400 °C	100 nm CdS film at 500 °C
29	101	3.1627	130	260	270
36	102	2.4507	100	165	170
43	110	2.0700	75	130	135
51.8	112	1.7620	70	106	108
52.8	201	1.7320	68	100	102
69	210	1.3551	60	98	100

CONCLUSION

The effects of thermal treatments on the vibrations of functional groups and optical properties of 100 nm CdS films for optoelectronics applications have been presented. Higher optical transmittances of about 90 % and relatively low absorbances were estimated for the films. The energy band gaps of 2.42, 2.4 and 2.9 eV were estimated for the as grown, 400 and 500 °C 100 nm CdS films. The annealing temperature has effect on the transmittance spectra of 100 nm CdS films at some specific wave numbers but their functional groups were unaltered. Based on the results obtained, 100 nm CdS film deposited via thermal evaporation and annealed at 400 °C is hereby encouraged for the development of CdS/CdTe polycrystalline thin film solar cells.

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