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Optimization of Thickness of Znte Thin Film As Back Contact for Cdte Thin Film Solar Cells

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Abstract - ZnTe thin films of different thickness ranging from 100nm to 500nm were prepared on glass substrate by thermal evaporation method. The effects of thickness on optical and structural properties of thin films were studied. AFM images indicated crystalline natureof ZnTe. XRD revealed that grain size increases with increase of film thickness. The internal strain and dislocation density decreased with increase in film thickness. The optical properties exhibited a decreasing trend of band gap from 2.25eV to 1.9eV with increase in thickness. Transmittance decreased as the thickness was increased and displayed 30% transmittance in the visible range at 300nm. Surface roughness increased up to 300nm after which it decreased. The results elucidate that ZnTe back contact of 300nm thickness is ideal and efficient to be used in CdTe solar cell.

1. INTRODUCTION

ZnTe, a II-VI semiconductor, is predominantly obtained in p-type form [1] and is widely used in modern technologies of opto-electronic devices (light-emitting diodes, solar cells, photo detectors, etc.) because of its excellent characteristics, such as large energy band gap 2.23–2.25eV, low resistivity, high transparency in visible spectral domain, etc. [2]. ZnTe when used as a back contact layer in CdTe/CdSe solar cells increases the fill factors > 0.76 and energy conversion efficiency by 12.9% [3]. ZnTe when used as an intermediate layer at metal/CdTe structures induces ohmic back contacts in CdS/CdTeheterojunction solar cells [4].

One of the most important applications of ZnTe is high efficiency stable electrical back contacts in CdTe based solar cells [5]. The study around this has been gaining interest in the recent past. Wu LiLi et al. have proposed ZnTe can be applied as a back-contact layer of CdTe solar cells due to small valence band offset with CdTe [6]. Though considerable reports on various properties of ZnTe viz. optical and electrical properties [7-9], photoconductivity [10], electrical resistivity [11-12] and conduction [13], etc. are available, but the studies on thickness dependent optical, electrical and structural properties are sparse. In the present work, we are reporting the optimization of thickness of ZnTe thin films with respect to its usage as a back contact layer for CdTe solar cells.

2. EXPERIMENTAL PART

Pure ZnTe (99.99%) material procured from Sigma Aldrich was used as source material. The films were prepared on glass substrate by thermal evaporation technique using a vacuum coating unit (Hind High Vacuum coating unit 12A4D). Glass substrates were cleaned with soap water followed by ultra-sonication under double distilled water. The source-substrate distance was maintained at 13.5 cm. Rotary drive was used to obtain the uniform coating. All the films were prepared at high vacuum (˜10^{-5}mbar) and rate of evaporation was maintained at 5 A°/sec. The samples were prepared at room temperature. The temperature controller thermocouple was used to measure the substrate temperature. The thickness and deposition rate were measured using the quartz crystal thickness monitor (DTM-101). The optical studies were performed using UV-VIS-NIR spectrophotometer (Ocean Optics, USA. Model No. USB4000-XR). The morphological studies were carried out using A-100-AFM, APE Research, Italy.

3. RESULTS AND DISCUSSION

3.1. Optical properties

The transmittance spectra of different thickness of ZnTe thin films ranging from 100nm to 500nm have been presented in Fig. 1. In the visible region, 500nm shows transmission of 47% whereas 300nm shows transmission of 30%. With increase in film thickness there is a decrease in transmission and this is due to increase in surface roughness [14].

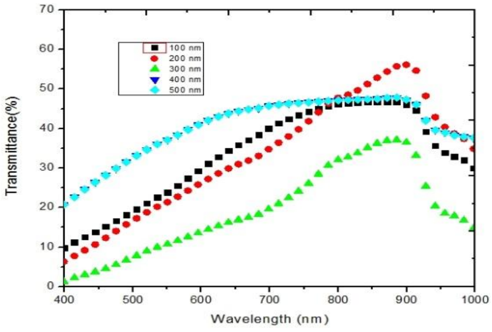

Fig 1. Transmittance spectra of ZnTe thin films of different thickness.

The absorption coefficient αcan be calculated using the relation [15],

$$\alpha = \left[\frac{2.303}{d}\right] \times \log\left(\frac{1}{T}\right)$$

The optical absorption spectra of ZnTe films deposited onto a glass is shown in Fig. 2. The optical absorbance was calculated from transmittance spectra for films of different thickness. The variation of optical absorbance with wavelength reveals a high absorption of energy at shorter wavelength and vice versa. The spectra also confirms that with increasing film thickness the absorption effect decreases exponentially as shown in Fig. 3. This is due to the effect of index of refraction of films [16]. The incident photon energy is higher than the band gap energy, due to which the electrons are excited from valence band into the conduction band. This generates electron-hole pairs and a new charge carrier distribution is created. This effect leads to rising of forward current when light of these wavelengths in visible region is illuminated [17]. The 300nm ZnTe thin film exhibits the absorption co-efficient is $7X10^6$ at 600nm wavelength, which is higher than the single crystal CdTe ($6 X 10^4$ at 600nm) [18]. This high absorption coefficient of 300nm film is very much useful in back contact application for CdTe solar cells.

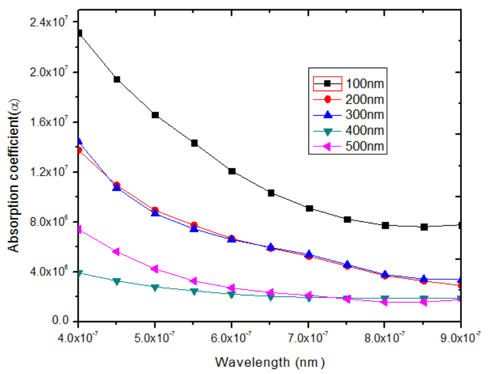

Fig2. Absorption co-efficient of ZnTe thin films of different thickness.

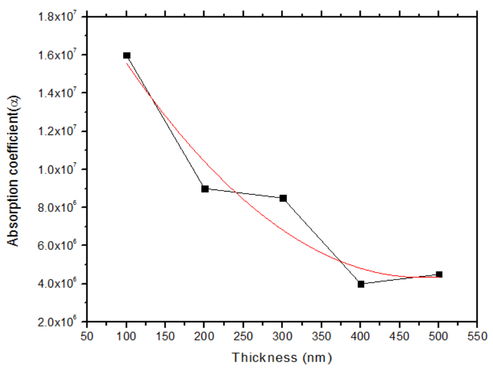

Fig 3.Absorption co-efficient of ZnTe thin films Vs thickness.

The optical band gap (Eg) was determined by analysing optical data with the expression for optical absorption coefficient α and photon energy hυ using the relation [15]

$$a = \frac{k(hv - Eg)^{n/2}}{hv}$$

where, k is a constant. A plot of $(\alpha h\upsilon)^2$ against hυ shown in Fig 4. is used to determine the band gap of ZnTe. Fig. 4a to 4d reveals that band gap of ZnTe is thickness dependent. Increase in film thickness results in decrease of energy band gap. With the increase in film thickness the individual levels of free atoms will broaden the energy bands and create overlapping levels. This occurs when atoms become closer to each other. Hence, with high film thickness there are several energy levels resulting in several overlapping energy bands in the band gap of these films. The overlapping energy bands therefore tend to reduce the energy band gap, resulting in lower band gaps for thicker films [19]. Fig.5.shows decrease in band gap with increasing film thickness from 2.25eV to 1.9eV. Rusu et al. have also reported optical band gap of ZnTe thin films to be between 2.40eV-1.95eV [20].

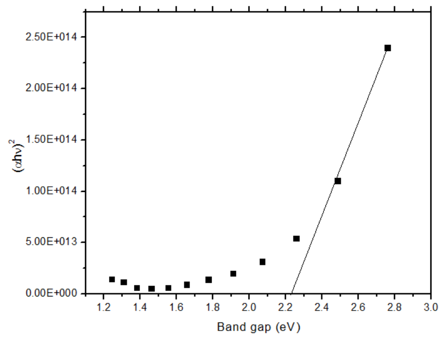

Fig. 4 a 100nm

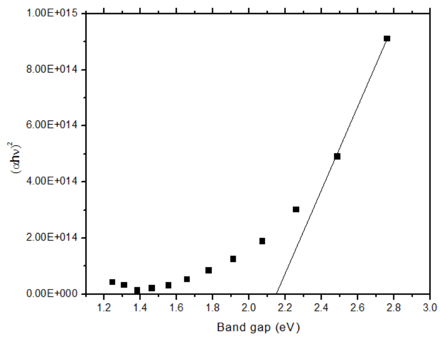

Fig. 4 b 200nm

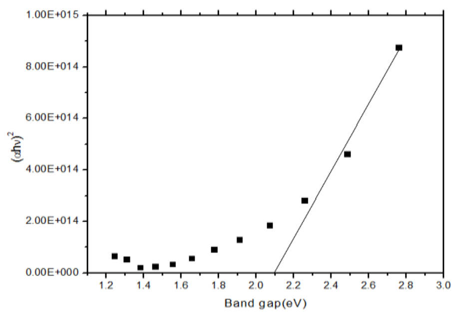

Fig. 4 c 300nm

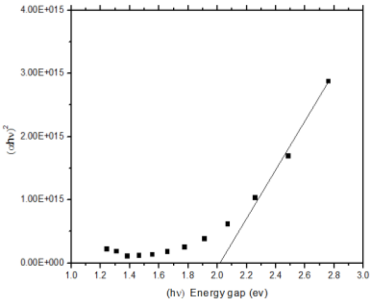

Fig. 4 d 400nm

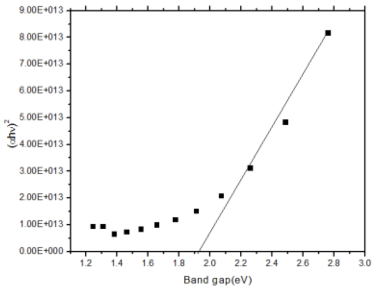

Fig. 4 e 500nm

Fig. 4 a) 100nm, b) 200nm c) 300nm d) 400nm e) 500nm Variation of $(\alpha h\nu)^2$ with photon energy for ZnTe films of different thickness.

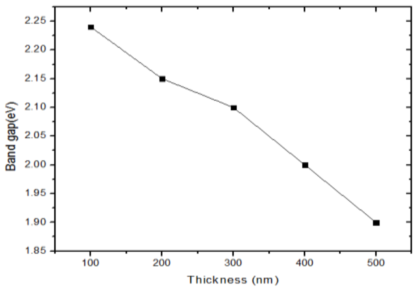

Fig. 5 Energy gap Vs thickness for ZnTe thin films.

3.2. Morphology

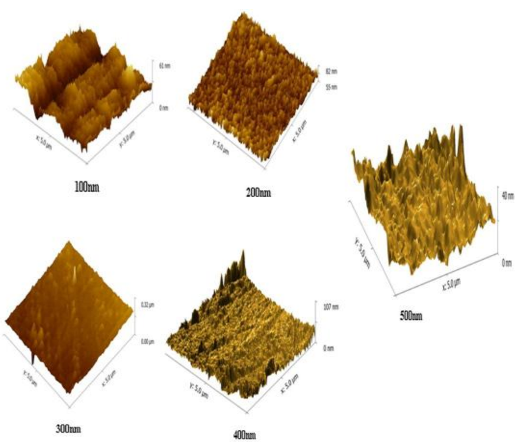

Fig. 6 Surface morphology of different thickness ofZnTe thin films

The three-dimensional AFM morphological images of deposited ZnTe film surface are shown in Fig. 6. The AFM morphology clearly reveals the deposition of ZnTe film took place with general thin film mechanism of nucleation growth. The films are found to be uniform and densely packed without any cracks or pinholes. However, the surface roughness found to vary for different thickness of the films. Fig. 7 illustrates root mean square value of surface roughness (rms roughness) which increases with increase in thickness. But after 300nm the roughness slowly starts decreasing. This may be due to aggregation of native grains into the larger clusters and also growth of some crystal planes (grain size) [21]. With increasing surface roughness the optical transmission decreases. Therefore, roughness is related to transmission which is one the prime requisites of the film for back contact application.

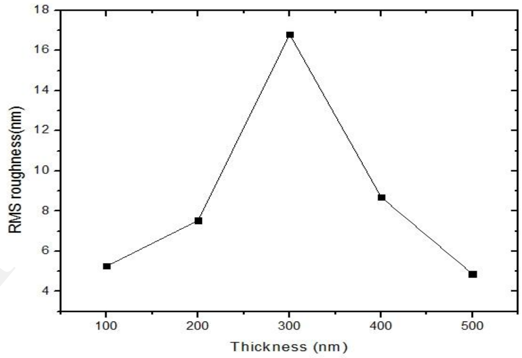

Fig. 7 Surface roughness of ZnTe thin films for different thickness.

3.3. Structural properties

The structure of ZnTe thin films of different thickness were analysed by X-ray diffraction technique as shown in Fig. 8. In ZnTe films only one prominent peak was observed at 2θ values of 25.8°preferably oriented along (111) plane. The films are crystalline in nature and have cubic structure as compared with Joint Committee on Powder Diffraction Standard [JCPDS File No. 80-

0022]data.

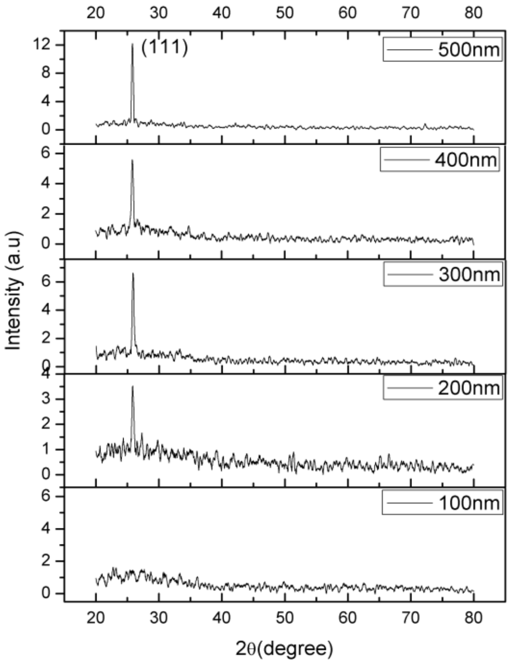

Fig. 8XRD of ZnTe thin films

The lattice parameters of the films were calculated using the Bragg's formula [15].

$$2d\sin\theta = n\lambda \qquad (1)$$

The grain size of the films was calculated from the XRD using Scherer's relation,

$$D = \frac{k\lambda}{\beta\cos\theta} \qquad (2)$$

Where, k is constant =0.94, λ is wavelength of radiation, β is full width half maxima and θ the diffraction angle.

The micro strain (ε) and dislocation density (δ) of films were estimated using the equations

$$\varepsilon = \frac{\beta\mathrm{Cos}\theta}{4} \qquad (3)$$

$$\delta = \frac{1}{D^2} \qquad (4)$$

The crystallite size (D), Strain (ε), dislocation density (δ) and lattice spacing are calculated and presented in Table1.

Sample (ZnTe nm)	2θ (degrees)	FWHM (radian)	Grain sizeD (nm)	Dislocation density δ(E+15 lin/m2)	Strain(lin-2 m-4) (E-3)
100	25.80	0.0108	14.158	4.988	10.224
200	25.86	0.0082	18.881	2.804	7.666
300	25.81	0.0033	46.281	0.466	3.127
400	25.88	0.0026	59.391	0.283	2.437
500	25.84	0.0019	80.374	0.154	1.801

Table 1. XRD analysis of ZnTe thin films

It is observed from XRD pattern of films that intensity of (111) peak and its grain size have increased slowly with increase of film thickness from 100 to 200nm, while it is increased sharply for film thickness from 300nm to 500nm. The small grain size was observed due to slow growth of crystallite. But large grain has been observed for film of thickness 300nm to 500nm because of fast growth of crystallite. The improvement in crystallinity is due to increased ability of adatoms to move towards stable sites in the lattice [22] and the same has been reported elsewhere [23, 24]. The strain in thin film which is defined by disarrangement of lattice created during their deposition and depends upon the deposition parameters. In the present study, the strain decreases with increase of ZnTe thin film thickness. Low strain indicates better lattice arrangement in films. The dislocation is imperfection in the crystal which is created during growth of thin film. The dislocation density decreases with increase of film thickness. The optimum grain size of 300nm thickness is best suited to be used for back contact.

3.4. Work Function

Work function ofZnTe thin films can be calculated using the equation [15],

$$\phi_m > E_g + \chi \qquad (5)$$

where, ϕ_m is metal work function, Eg is band gap of semiconductor and 'χ' is electron affinity of semiconductor. The equation signifies that work function of metal should be greater than that of semiconductor (ZnTe/Se or Au) [25]

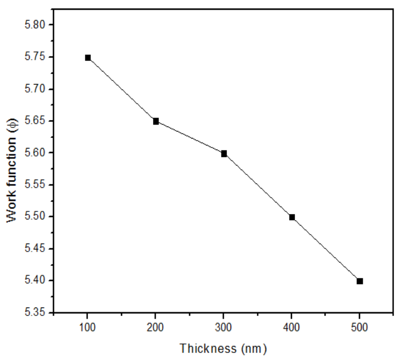

Fig. 9.Calculated work function Vs thickness.

The calculated work function with varying thickness is depicted in Fig. 9. As seen in the graph, ZnTe with thickness of 100nm has maximum work function of 5.75. It can be interpreted from the graph that work function decreases linearly with increasing film thickness. The 300nm ZnTe thin film has work function of 5.6 which is lower compared to CdTe work function of 5.8. This low work function of ZnTe thin film helps to form ohmic contact in CdTe solar cells.

4. CONCLUSION

ZnTe thin films were prepared using thermal evaporation method for different thickness (100-500nm). The structural, optical and morphological properties of thin films were studied in the visible region. Based on the results, the 300nm ZnTe thin film showed low transmittance in visible wavelength with maximum absorption coefficient, optimum surface roughness, appropriate band gap and work function. These results strongly support the use of ZnTe thin film as a back contact for CdTe solar cells.

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