

# Optimization of thickness of $\text{Sb}_2\text{Te}_3$ thin film as back contact for CdTe thin film solar cells

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## ABSTRACT

$\text{Sb}_2\text{Te}_3$  thin films of different thickness ranging from 100 to 500 nm were prepared on glass substrate by thermal evaporation method. The effects of thickness on structural, optical and electrical properties of thin films were studied. XRD revealed that grain size increases from 1.1nm to 98.7 nm with increase in film thickness. The internal strain and dislocation density decreased with increase in film thickness. The optical band gap decreases from 1.3 to 0.9 eV with increase in film thickness. AFM images indicated crystalline nature of  $\text{Sb}_2\text{Te}_3$ . Surface roughness increased up to 400nm after which it decreased. The resistivity decreases with increase in thickness at room temperature ranging from  $2.9 \times 10^{-3}$  to  $1.35 \times 10^{-4}$   $\Omega\text{cm}$ . The work function and barrier height decreases as the film thickness increases from 5.45 to 5.05eV and barrier height from 0.3 to -0.1eV. The results elucidate that  $\text{Sb}_2\text{Te}_3$  back contact of 400 nm thickness is ideal and efficient to be used in CdTe solar cell. Copyright © 2014 VBRI press.

**Keywords:** Antimony telluride;  $\text{Sb}_2\text{Te}_3$ ; thermal evaporation; optical band gap; work function; electrical characteristics.



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## Introduction

$\text{Sb}_2\text{Te}_3$ , a chalcogenide, is a binary compound of the form  $\text{A}_2\text{VB}_3\text{VI}$  having a narrow band gap of  $E_g \sim 0.2\text{eV}$  [1]. Investigations on  $\text{Sb}_2\text{Te}_3$  have been carried out for its semiconductor properties viz. high Seebeck coefficient, low thermal conductivity, low electrical resistivity, low band gap and long-term stability and the results of the same have been reported elsewhere [2]. Because of these characteristics it has found its applications in numerous areas like television cameras with photo-conducting targets, infrared spectroscopy, electronic and optoelectronic devices and thermoelectric devices [3]. One of the crucial applications of  $\text{Sb}_2\text{Te}_3$  is high efficiency stable electrical back contacts for CdS/CdTe based solar cells. There are many back contact materials available today, of which Cu or even materials doped with Cu have been used to form back contacts, such as ZnTe:Cu, Cu/Au, Cu/graphite, and Cu/Mo [4]. But, these suffer with few limitations. Cu-diffusion in CdTe is very rapid and extends deep into the absorber, thereby affecting the stability of the device considerably. Therefore, Cu-free alternative back contact materials like  $\text{Sb}_2\text{Te}_3$  can be embraced [5]. Fabrication of CdS/CdTe solar cell using  $\text{Sb}_2\text{Te}_3$  thin film as a back contact has been reported elsewhere. These solar cells have shown high efficiency of 14.6% and long-term device stability [6].

Considerable reports on various properties of  $\text{Sb}_2\text{Te}_3$  viz. optical and electrical properties, photoconductivity,

electrical resistivity and conduction, etc. are available, but the studies on thickness dependent optical, electrical, structural, I-V properties are sparse. In the present work, we are reporting the thickness dependent properties of the prepared samples and also optimization of thickness of  $\text{Sb}_2\text{Te}_3$  thin films with respect to its usage as a back contact layer for CdTe solar cells.

## Experimental

### Substrate preparation

In the present work, Blue-Star glass slides were used. The glass substrates were cleaned with soap solution. The substrates were then subjected to ultra-sonication for 3 min for 3 times in Acetone and then in double distilled water for 3 min. for 3 times. The substrates were dried using hot air drier and finally wiped using Acetone.

### Film preparation

Pure  $\text{Sb}_2\text{Te}_3$  (99.99%) material procured from Sigma Aldrich was used as source material. Thin films of different thickness were prepared on glass substrate by thermal evaporation technique using a vacuum coating unit (Hind High Vacuum coating unit 12A4D). The source-substrate distance was maintained at 13.5cm. Rotary drive was used to obtain the uniform coating. All the films were prepared at high vacuum ( $\sim 10^{-5}$ mbar) and rate of evaporation was maintained at 5  $\text{\AA}/\text{sec}$ . The samples were prepared at room temperature. All films were annealed at 200 $^\circ\text{C}$  for 3 hours in ambient air.

### Measurements

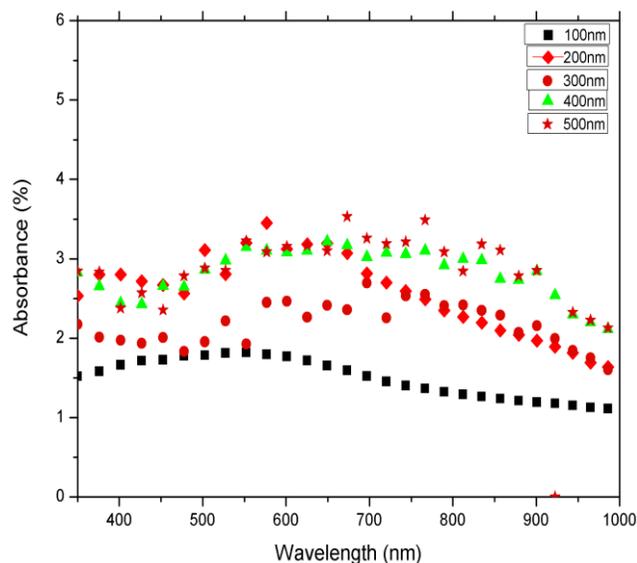
The temperature controller thermocouple was used to measure the substrate temperature. The thickness and deposition rate were measured using the quartz crystal thickness monitor (DTM-101). The optical studies were performed using UV-VIS-NIR spectrophotometer (Ocean Optics, USA. Model No. USB4000-XR). The morphological studies were carried out using A-100-AFM, APE Research, Italy. Structural properties were studied using PANalytical system having  $\text{CuK}\alpha$  radiation ( $\lambda = 1.54 \text{ \AA}$  with  $2\theta = 20^\circ - 80^\circ$ ). I-V characteristics of as-grown samples were recorded using Keithley instrument (Model No: 2602A). I-V was performed at room temperature.

## Results and discussion

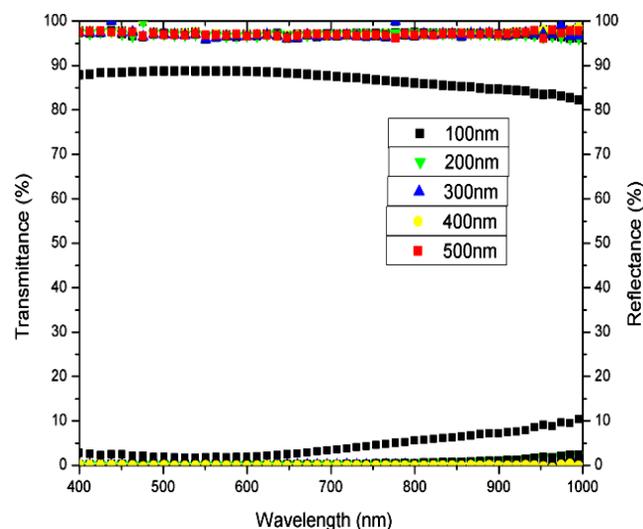
### Optical properties

The optical absorbance spectra of  $\text{Sb}_2\text{Te}_3$  thin films, having different thickness of 100-500nm, are shown in **Fig. 1**. The absorbance at the wavelength 600nm reveals average absorbance of 2.9%. These spectra reveal that overall absorbance increases with increase in thickness. This is because thicker films have more atoms present leading to more availability of states for the photons to be absorbed [7]. **Fig. 2** illustrates the transmittance spectra of different thickness of  $\text{Sb}_2\text{Te}_3$  thin films ranging from 100nm to 500nm. In the visible region (400 - 800nm), the 100nm thickness of the film transmission is 0.5%. The transmission shows a decreasing trend with increase in film

thickness because of increase in surface roughness [8]. For 400nm thickness, in the visible region (400nm-800nm) there is no transmission, therefore making it suitable for its usage as back contact application.



**Fig. 1.** Absorbance spectra of  $\text{Sb}_2\text{Te}_3$  thin films of different thickness.



**Fig. 2.** Transmittance and reflectance spectra of  $\text{Sb}_2\text{Te}_3$  thin films of different thickness.

The reflectance of the films was calculated from transmittance and absorbance values using the expression [7]:

$$A + T + R = 1$$

$$R = 1 - (A + T) \quad (1)$$

A reflectance of 97% was achieved in the visible region (400nm-800nm). However, the average reflectance was found to be 96.5% irrespective of the thickness of the films. The high reflectance and low transmission and absorption satisfy the criteria required for an efficient back contact for CdTe based solar cell. This can be observed at a film thickness of 400nm.

The optical band gap ( $E_g$ ) was determined by analyzing optical data with the expression for optical absorption coefficient  $\alpha$  and photon energy  $h\nu$  using the relation [9],

$$\alpha = \frac{k(h\nu - E_g)^{n/2}}{h\nu} \quad (2)$$

where,  $k$  is constant. A plot of  $(\alpha h\nu)^{1/2}$  versus  $h\nu$  shown in Fig. 3 is used to determine the band gap of  $Sb_2Te_3$ . It is found that band gap of  $Sb_2Te_3$  is thickness dependent. Optical measurement indicates that there is an indirect transition having an energy gap of 1.3eV to 0.9eV. The increase in film thickness results in decrease of energy band gap as shown in Fig. 4. This is due to the crystallite size-dependent properties of the energy band gap [10].

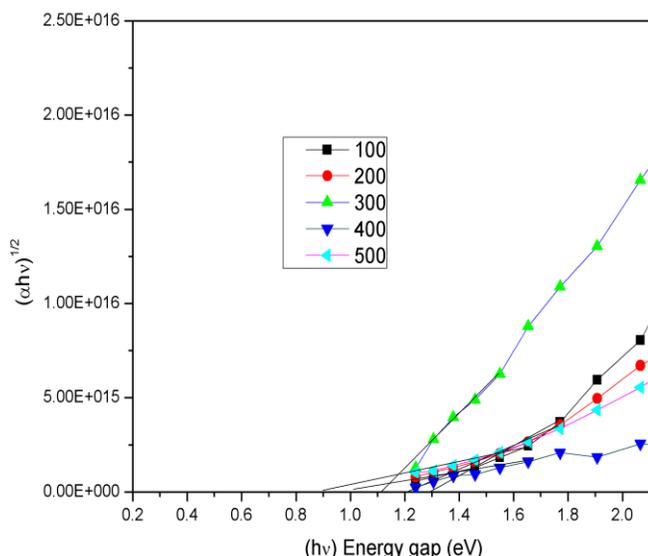


Fig. 3. Variation of  $(\alpha h\nu)^{1/2}$  against  $h\nu$  for  $Sb_2Te_3$  thin films of different thickness.

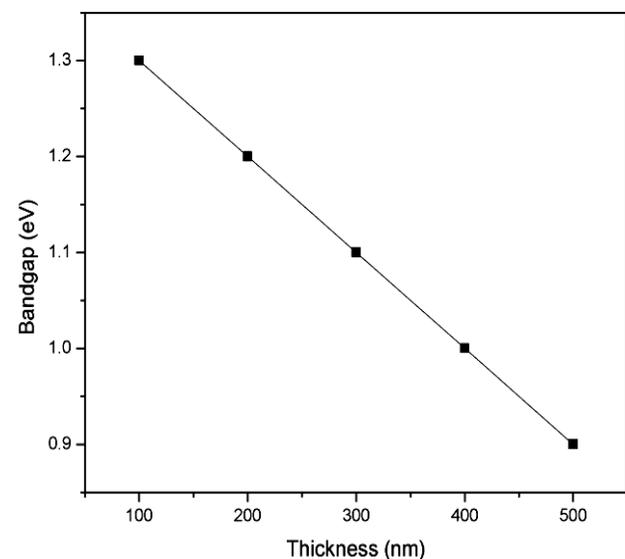


Fig. 4. Energy gap Vs thickness of  $Sb_2Te_3$  thin films.

Work function of  $Sb_2Te_3$  thin films can be calculated using the equation [9],

$$\phi_m > E_g + \chi \quad (3)$$

where,  $\phi_m$  is metal work function,  $E_g$  is band gap of semiconductor and ' $\chi$ ' is electron affinity of semiconductor. The equation signifies that work function of metal needs to be greater than that of semiconductor ( $Sb_2Te_3/Ni$ ) [11].

The calculated work function with varying thickness is depicted in Fig. 5.  $Sb_2Te_3$  with thickness of 100nm has maximum work function of 5.45eV. The work function decreases linearly with increase in film thickness. The 400nm  $Sb_2Te_3$  thin film has work function of 5.16eV which is lower compared to that of CdTe which is 5.8eV therefore making it suitable to be used as a back contact for CdTe solar cells.

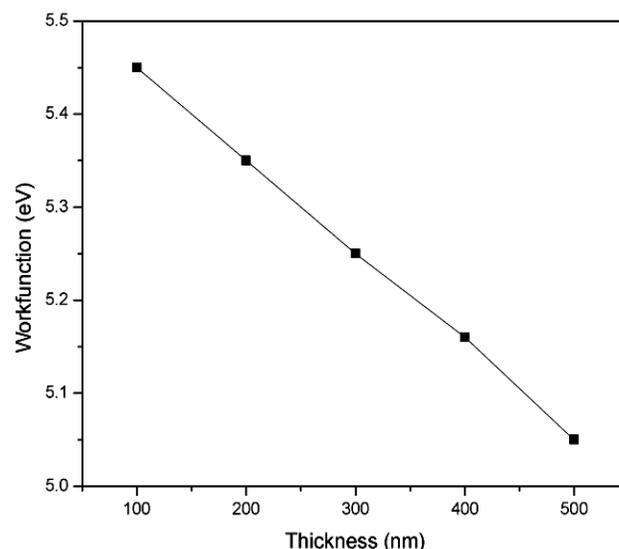


Fig. 5. Calculated work function Vs thickness.

Barrier height of  $Sb_2Te_3$  thin films can be calculated using the equation [12],

$$\phi_b = \phi_s - \phi_m \quad (4)$$

where,  $\phi_s$  is work function of semi-conductor and  $\phi_m$  work function of metal. During normal device operation (i.e. at forward bias under illumination), majority carriers will be moving from CdTe to metal. Most of the metals do not have high work function. In p-type, holes will encounter a barrier over which they must pass via a thermionic emission process. The height of the barrier will be equal to the difference of two work functions. The presence of back-contact barrier can significantly affect the current-voltage characteristics of CdTe based solar cells, primarily by impeding hole transport. A zero or a negative value back barrier height is preferred for ohmic contact for CdTe based solar cell [11]. As depicted in Fig. 6, as the film thickness of 400 nm having a barrier height of 0.01eV is appropriate to be used as a back contact for CdTe based solar cell.

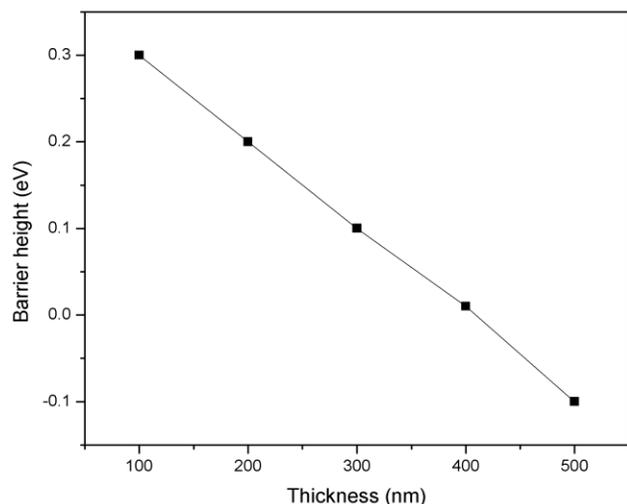


Fig. 6. Barrier height vs thickness.

### Structural properties

The structure of  $\text{Sb}_2\text{Te}_3$  thin films of different thickness were analyzed by X-ray diffraction technique as shown in Fig. 7. In the 100nm film thickness only one peak was observed at  $2\theta$  values of  $38.38^\circ$  preferably oriented along (1010) planes. Film thickness of 200nm-400nm showed two peaks at  $28.77^\circ$  (015) and  $38.84^\circ$  (1010). But 500nm film thickness showed 6 peaks at  $2\theta$  values of  $28.70^\circ$ ,  $38.78^\circ$ ,  $42.76^\circ$ ,  $45.11^\circ$ ,  $46.38^\circ$ ,  $54.63^\circ$ . These peaks correspond to (009), (015), (1010), (110), (0015), (116), (027) respectively.  $\text{Sb}_2\text{Te}_3$  thin film show rhombohedral structure when compared with JCPDS card [72-1990]. With increase in film thickness the intensity increases, this is due to improvement in crystallinity of the films and growth in grain size as the film thickness is elevated.

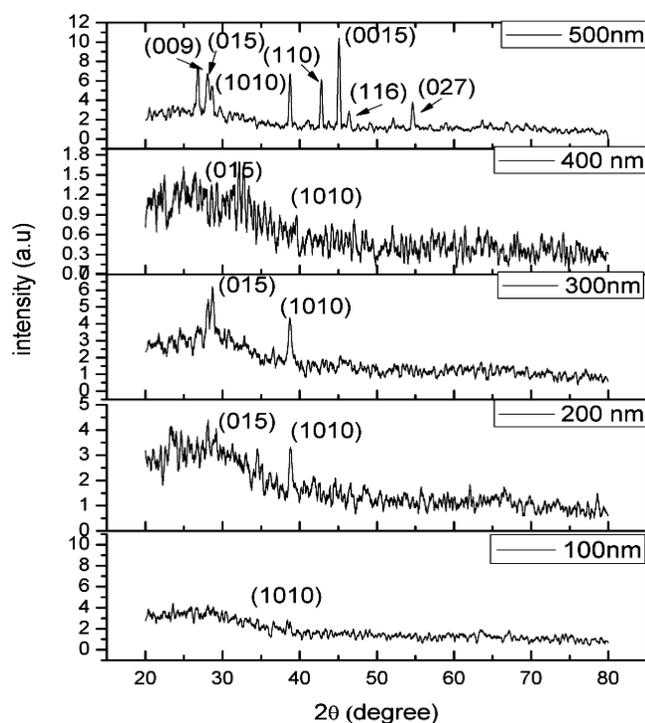


Fig. 7. XRD of  $\text{Sb}_2\text{Te}_3$  thin films.

The lattice parameters of the films were calculated using the Bragg's formula [13].

$$2d \sin \theta = n\lambda \quad (5)$$

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

$$D = \frac{k\lambda}{\beta \cos \theta} \quad (6)$$

where,  $k$  is constant = 0.94,  $\lambda$  is wavelength of radiation,  $\beta$  is full width half maxima and  $\theta$  the diffraction angle. The micro strain ( $\epsilon$ ) and dislocation density ( $\delta$ ) of films were estimated using the equations.

$$\epsilon = \frac{\beta \cos \theta}{4} \quad (7)$$

$$\delta = \frac{1}{D^2} \quad (8)$$

The crystallite size ( $D$ ), Strain ( $\epsilon$ ), dislocation density ( $\delta$ ) and lattice spacing are calculated and presented in Table 1.

Table 1. XRD analysis of  $\text{Sb}_2\text{Te}_3$  thin films.

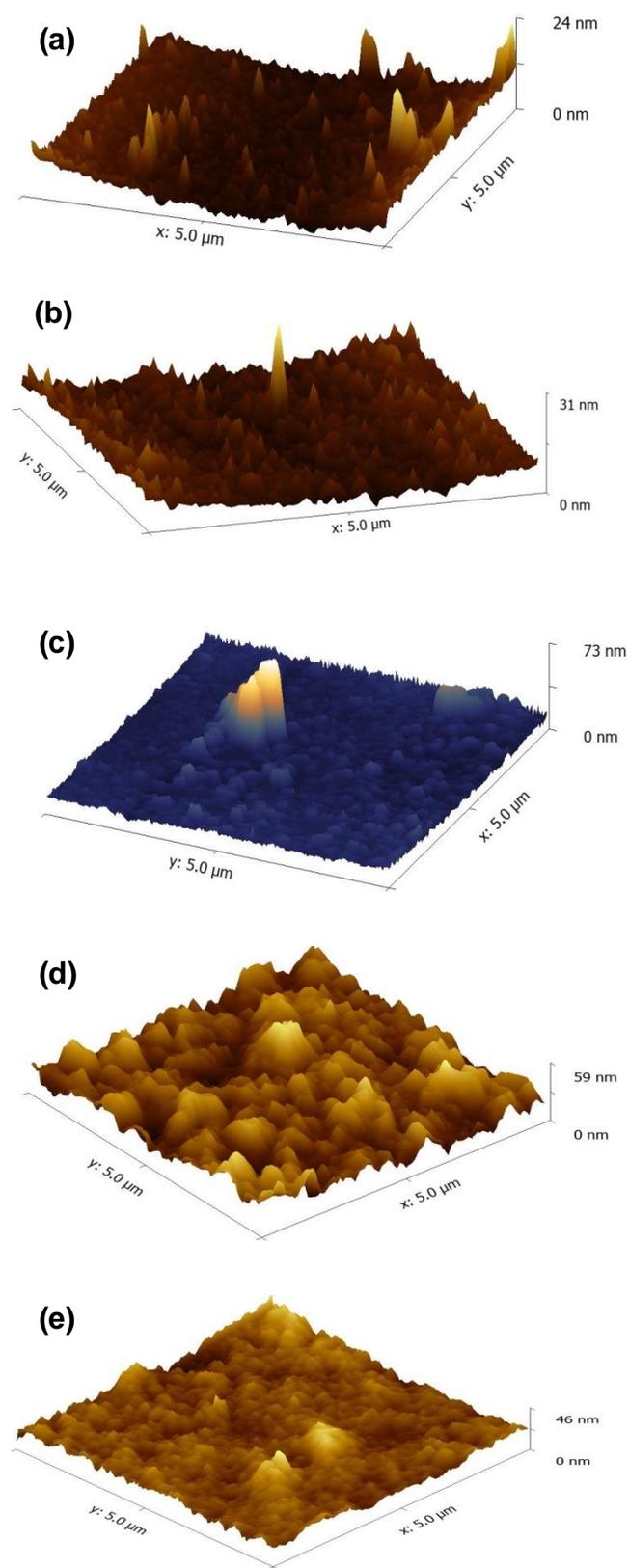
Sample ( $\text{Sb}_2\text{Te}_3$ nm)	$2\theta$ (degrees)	FWHM (radian)	Grain size D (nm)	Dislocation density $\delta$ ( $\text{E} + 15 \text{ lin}/\text{m}^2$ )	Strain ( $\text{lin}^{-2} \text{ m}^{-4}$ ) ( $\text{E}^{-3}$ )
100	38.38	0.1317	1.165	736.22	124.209
200	38.84	0.0879	1.956	261.36	74.007
300	38.70	0.0164	10.014	9.9710	14.455
400	38.85	0.0041	41.891	0.5698	3.455
500	38.78	0.0017	98.700	0.1026	1.466

There is a growth in the grain size as the film thickness is elevated from 100nm to 200nm. The small grain size was observed due to slow growth of crystallite. It amplifies sharply for film thickness from 300nm to 500nm. This is because of rapid growth of crystallite. The improvement in crystallinity is due to increased ability of adatoms to move towards stable sites in the lattice [13]. The strain in thin film which is defined by disarrangement of lattice created during their deposition and depends upon the deposition parameters. The strain decreases with increase of  $\text{Sb}_2\text{Te}_3$  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 400nm thickness is best suited to be used for back contact.

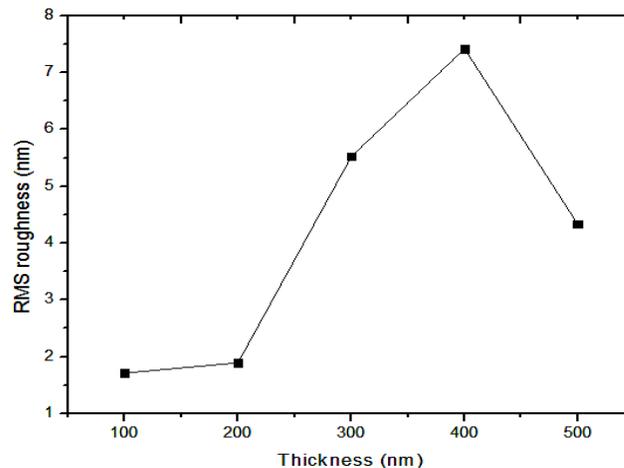
### Morphology

AFM images of  $\text{Sb}_2\text{Te}_3$  thin films of thickness 100nm to 500nm are shown in Fig. 8. It can be found from Fig. 8 that the films are fully covered, homogeneous, well adherent and free from crystal defects such as pin hole and cracks. Fig. 9 illustrates that root mean square value of surface roughness (rms roughness) increases up to 400 nm thickness, after which roughness decreases with increasing thickness. This may be due to aggregation of native grains into the larger clusters and also growth of some crystal

planes (grain size) [14]. With increasing surface roughness the optical transmission decreases. Therefore, roughness is related to transmission which is one of the prime requisites of the film for back contact application.



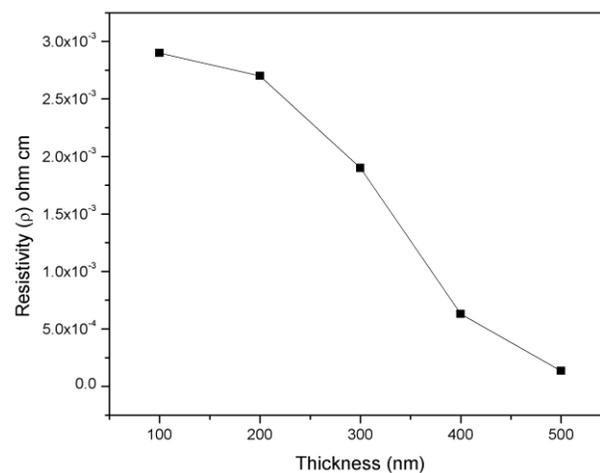
**Fig. 8.** Surface morphology of different thickness (a) 100 nm, (b) 200 nm, (c) 300 nm, (d) 400 nm and (e) 500 nm, of  $\text{Sb}_2\text{Te}_3$  thin films.



**Fig. 9.** Surface roughness of  $\text{Sb}_2\text{Te}_3$  thin films for different thickness.

### Electrical properties

As shown in **Fig. 10**, the electrical resistivity of  $\text{Sb}_2\text{Te}_3$  thin films at room temperature shows a decreasing trend from  $3 \times 10^{-3}$  to  $1.35 \times 10^{-4} \Omega \text{ cm}$  with increase in film thickness. This is due to islands of aggregated particles with lot of insulating gaps in very thin films. As thickness increases the islands of aggregated particles transform into continuous bands thereby minimizing the insulating gaps. Ultimately resistivity of thin film decreases with increase in thickness [15]. The 400nm  $\text{Sb}_2\text{Te}_3$  thin film has resistivity of  $5 \times 10^{-4} \Omega \text{ cm}$  compared to p-type CdTe single crystal whose resistivity is on the order of  $10^7 \Omega \text{ meter}$  [16].



**Fig. 10.** Resistivity Vs thickness of  $\text{Sb}_2\text{Te}_3$  thin films.

### Conclusion

In summary, thickness dependent properties were studied and optimization of thickness of  $\text{Sb}_2\text{Te}_3$  thin film as back contact for CdTe solar cells was carried out.  $\text{Sb}_2\text{Te}_3$  thin films were prepared using thermal evaporation method for different thickness (100-500nm). The optical properties exhibits low transmission, high reflection, medium absorption and decrease in band gap with increasing thickness. The structural analysis indicates the films are crystalline and growth in grain size with increase in thickness. The morphology of thin films shows elevation in

surface roughness as the thickness increases. Resistivity reduces with increase in thickness. Work function and barrier height drops with increase in thickness. It was observed that 400nm film thickness shows more optimum characteristics compared to other thickness as there is a sharp increase in grain size and high surface roughness, due to which the transmission is low and reflection is high in the visible wavelength. These are the prominent characteristics of a back contact. All these properties indicate that  $\text{Sb}_2\text{Te}_3$  thin films can be considered to be used for device applications as well as back contact material for CdTe solar cells.

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