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Temperature Dependent Optical and Morphological Properties of Sb_2Te_3 Thin Films

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Abstract— **Sb_2Te_3 thin films of different temperature ranging from room temperature to 200°C were prepared on glass substrate by thermal evaporation method. The effects of temperature on optical and morphological properties of thin films were studied. AFM images indicated crystalline nature of Sb_2Te_3. The optical properties exhibited a decreasing trend of band gap from 1.24eV to 1.06eV with increase in temperature. Transmittance decreased as the temperature was increased and displayed no transmittance in the visible range at 200°C. Surface roughness decreased up to 150°C after which it increased.**

Keywords— **Sb_2Te_3, thermal evaporation, optical band gap, AFM.**

I. INTRODUCTION

Antimony telluride (Sb_2Te_3) is a binary p-type semiconductor and has a narrow band gap with Eg ~0.3eV [1]. Sb_2Te_3 has been widely used in industrial applications such as target material in television camera, microwave devices, switching devices, thermoelectric devices and optoelectronic devices due to its attractive photo conducting properties and its high Seebeck coefficient, low thermal conductivity, low electrical resistivity, low band gap, and long-term stability [2]. In optoelectronic devices it is used as a back contact to CdTe based solar cells mainly because it offers long term stability and is Cu-free. An efficiency of 14.6% for CdTe solar cells with Sb_2Te_3 has been realized [3].

Different methods have been used to prepare Sb_2Te_3 thin films, such as thermal evaporation [4], atomic layer epitaxy (ALE) [5], sputtering [6, 7], electrochemical method [8], flash evaporation [9] and metal organic chemical vapor deposition (MOCVD) [10]. Among all these techniques, thermal evaporation offers several advantages in the growth of Sb_2Te_3 thin films for CdTe solar cells, such as simple evaporation equipment, and a relatively short fabrication processing time.

In this work, Sb_2Te_3 thin films were prepared through thermal evaporation method, and the effect of different substrate temperatures on optical and morphological properties with respect to its usage as a back contact layer for CdTe solar cells were investigated.

II. EXPERIMENT

Pure Sb_2Te_3 (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 13.5cm. 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, 100°C, 150°C, 200°C. The temperature controller thermocouple was used to measure the substrate temperature. The film thickness was 100nm 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.

III. RESULT AND DISCUSSION

A. Optical Properties

The transmittance spectra of different temperature of Sb_2Te_3 thin films ranging from room temperature to 200°C is illustrated in Figure 1.

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In the visible region (400nm-800nm), the transmission presents a decreasing trend with increase in temperature because of the fact that when substrate temperature is elevated, the films becomes crystalline which creates grain boundaries and consequently less absorbance and more reflectance, which in turn causes a drop in transmittance.

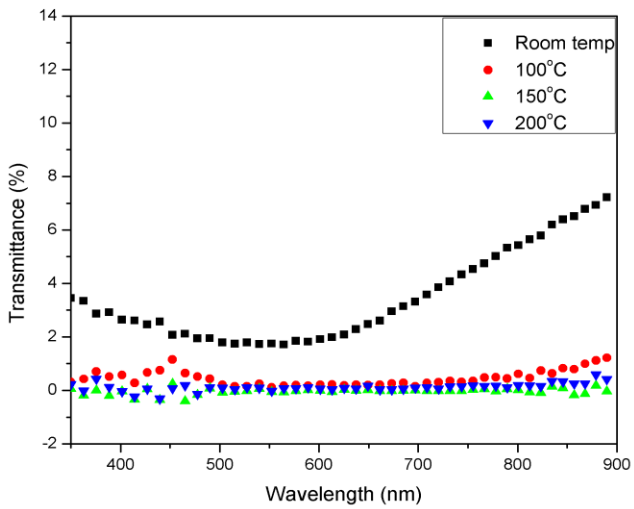

Figure 1: Transmittance spectra of Sb_2Te_3 thin films of different temperature

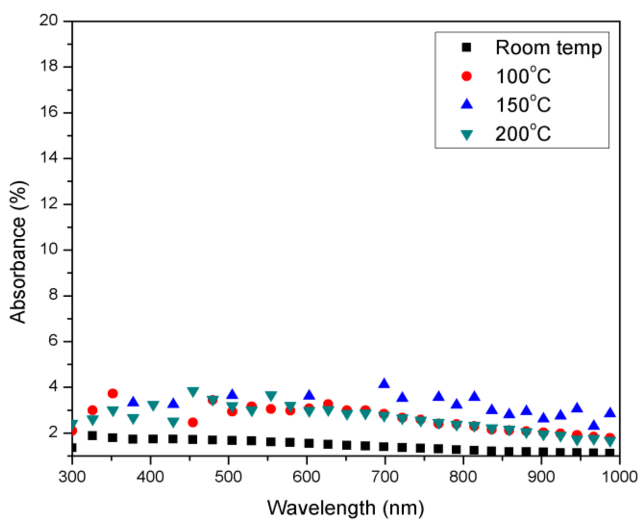

Figure 2: Absorbance spectra of Sb_2Te_3 thin films of different temperature

The variation of optical absorbance with wavelength for Sb_2Te_3 thin films grown at different substrate temperatures is displayed in figure 2. In all cases it is observed that the absorption in between 2%-3% at all temperatures. This consequently implies a marginal improvement in the reflection of the films.

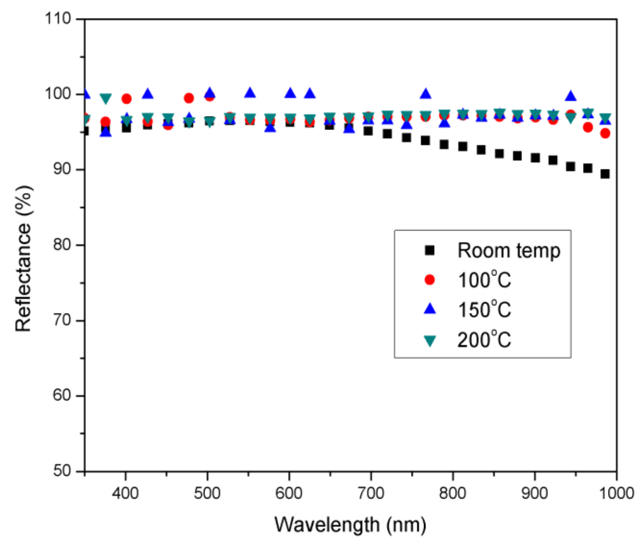

Figure 3: Reflectance spectra of Sb_2Te_3 thin films of different temperature

The reflectance of the films was calculated from transmittance and absorbance values using the expression [4]:

$$A + T + R = 1$$

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

$$A = 100 - (R + T)(in\ \%) \quad (2)$$

A reflectance of 96% was achieved in the visible region (400nm-800nm). However, the average reflectance, irrespective of the temperature of the films was found to be same as 96%. The remaining 3% absorbance enhances the mobility of the carriers. High reflectance, low absorption and low transmission are the primordial requisite of an efficient for photovoltaic back contacts. The optical results satisfy the criteria required for an efficient back contact.

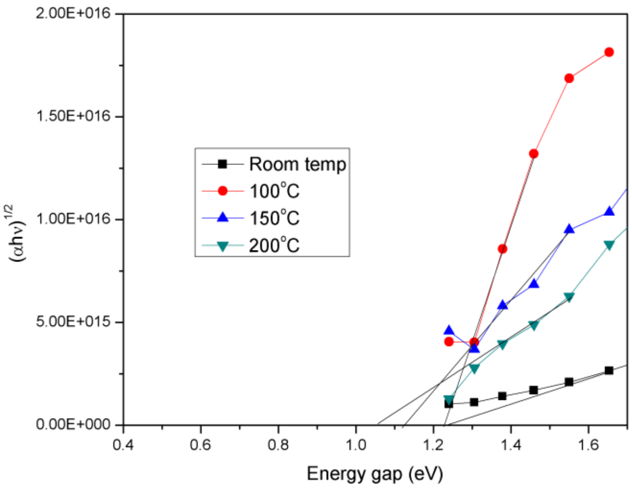

Figure 4: Variation of $(\alpha h\upsilon)^{1/2}$ against hυ for Sb_2Te_3 thin films of different temperature.

The optical band gap (E_g) was determined by analysing optical data with the expression for optical absorption coefficient α and photon energy hυ using the relation [4]

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

Where, k is a constant. A plot of $(\alpha h\upsilon)^{1/2}$ versus hυ shown in Figure 4 is used to determine the band gap of Sb_2Te_3. It is found that band gap of Sb_2Te_3 is temperature dependent. Optical measurement indicates that there is an indirect transition having an energy gap is 1.24eV to 1.06eV. As depicted in Figure 4, the energy band gap is reduced as the substrate temperature intensifies. This is due to enlargement of particle size and lowering of strain and dislocation density [4].

B. Morphology

AFM images of Sb_2Te_3 thin films of temperature ranging from room temperature to 200°C are shown in Figure 5 which reflects that the Sb_2Te_3 deposited is uniform and densely packed, homogeneous, well adherent and free from crystal defects such as pin hole and cracks. Figure 6 illustrates that root mean square value of surface roughness (rms roughness) decreases up to 150°C, this may be due to increased grain density causing uniform distribution on the film's surface, after which roughness enhances with increasing substrate temperature which may be due to diffusion of some grains thereby forming clusters, which results in increase of rms roughness of the film's surface [11].

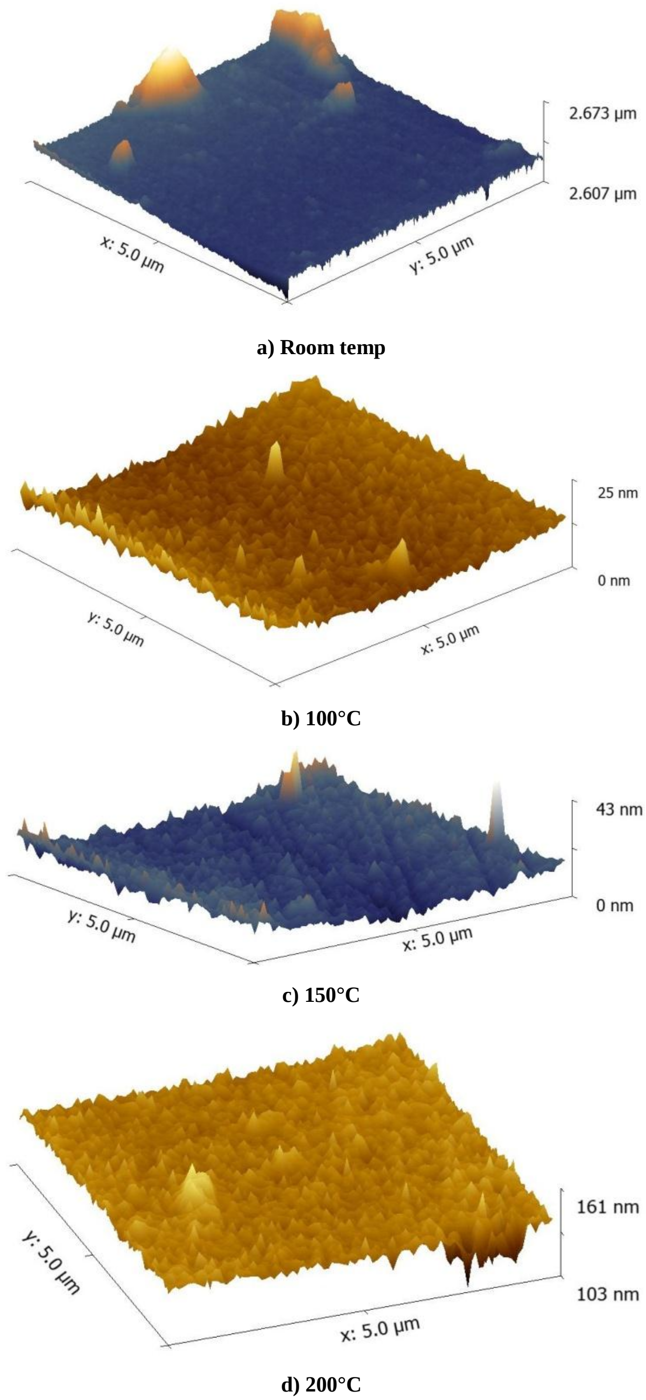

Figure 5: Surface morphology of Sb_2Te_3 thin films for different temperature.

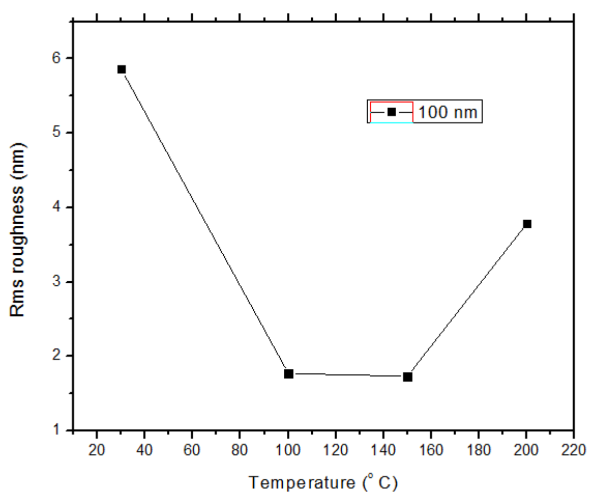

Figure 6: Surface Roughness of Sb_2Te_3 thin films for different temperature.

IV. CONCLUSION

Antimony Telluride thin films were deposited at different temperatures using thermal evaporation method. The optical properties of the thin films show that there is a small variation in transmittance and reflectance and the band gap varies from 1.24eV to 1.06eV with increase in substrate temperature from RT to 200°C, respectively, due to the improvement in the crystallization of the film. The surface roughness increases as observed by AFM measurement. This result makes it evident that Sb_2Te_3 thin films can be used in photovoltaic application.

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