INVESTIGATION OF OPTICAL PROPERTIES OF Sb_2S_3 THIN FILMS

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Abstract. *Thin films of Sb_2S_3 have been deposited by vacuum evaporation technique onto highly cleaned glass substrates under vacuum of the order 10^{-5} torr. The structure of the films was determined by their X-ray diffraction patterns and AFM images. Transmittance measurements in the wavelength range (500-1100 nm) were used to compute the refractive index using the Swanepoel's method. The optical properties of these thin films have been investigation from transmission spectra by using Wemple-DiDomenico single oscillator model. These films posed, in general good transparency, exhibiting an interference pattern. The wavelength dependence of refractive index and extinction coefficient of these films has been reported.*

Keywords: *thin films, optical properties, single oscillator model.*

1. INTRODUCTION

The knowledge of the optical properties of thin films is very important in many scientific, technological and industrial applications of thin films such as photoconductivity, solar energy, photography and numerous other applications. Study of optical absorption has been one of the most productive methods in understanding the band structure and energy gap of both crystalline and amorphous materials. The measurement of optical absorption coefficient, particularly near the fundamental absorption edge is a standard method for the investigation of optical properties.

Antimony trisulfide is a V_2-VI_3 compound, which could be prepared using different methods such as chemical deposition [1-3], spray pyrolysis [4, 5], electrodeposition [6, 7] and vacuum evaporation [8-10]. The Sb_2S_3 thin films have many applications in electronics and optical information storage [11]. The optical constants of the Sb_2S_3 thin films are, obviously, of particular significance in most of film applications. As to the method for determining the optical constants of the thin films, we must consider that, if the thickness of film is sufficient to generate several interference fingers, it is possible to calculate the refractive index and the transmission spectrum alone [12].

2. EXPERIMENTAL

Sb_2S_3 thin films have been prepared onto glass substrates by thermal evaporation under vacuum ($p=2\times10^{-5}$ torr) of Sb_2S_3 high purity polycrystalline powder (99.99 % purity). Powdered material was heated in a quartz crucible to temperatures near the melting point of Sb_2S_3; it evaporated and condensed on glass substrates. The glass substrates had been previously cleaned and were kept at room temperature (T_S=300 K) during the deposition.

The substrates were mounted directly over the quartz crucible with about 10 cm separation. The Sb_2S_3 powder was evaporation with deposition rate of about 2 nm/s. The thickness, d, of thin films was determined by Fizeau's method for fringes of equal thickness [13] using an interferential microscope MII-4 (type Linnik). The thickness of the films was estimated to be around 0.20 μm.

Structural analysis of the Sb_2S_3 thin films was made using a Dron 3 X-ray diffractometer with CuK_α radiation (λ=1.5418 Å) at 40 kV and 30 mA in the scanning angle (2θ) from 20° to 60° with the scanning speed of 0.05 deg/s.

The surface morphology and roughness were examined by atomic force microscopy using atomic force microscopy (AFM) under ambient condition. The optical transmission spectra of the as-deposited and annealed films were recorded using a Perkin-Elmer Lambda 35 UV-VIS double-beam spectrophotometer in the wavelength range 400-1100 nm. The observed transmittance data were corrected relative to optically identical uncoated glass substrate. The transmission spectrum curve was used for calculating the optical constants of the investigated samples.

3. RESULTS AND DISCUSSION

X-ray diffraction pattern (XRD) was used to study the structure properties of Sb_2S_3 thin films. Fig. 1(a) shows a typical XRD pattern derived for the as- deposition thin film samples. The figure declares the absence of any sharp diffraction lines, indicating that amorphous nature of antimony trisulfide in thin film form. Fig. 2(b) shows an atomic forte microscopy (AFM) imaged picture of the surface of deposited Sb_2S_3 thin film. The surface of thin film was highly smooth. The average surface roughness of the film was around 4.5 nm and the thickness of the film estimated from AFM image was around 0.2 μm.

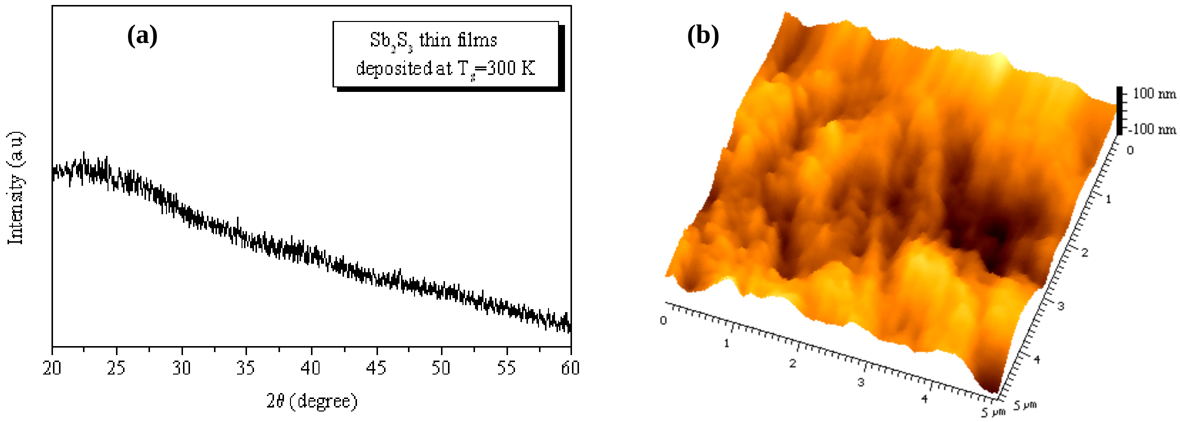

Fig. 1. (a) XDR pattern and (b) AFM image of Sb_2S_3 thin film deposited at 300 K.

The transmission spectrum in the wavelength range 500-1100 nm was used to calculate the optical constants of Sb_2S_3 thin films. Fig. 2(a) shows the transmission spectrum obtained for investigated sample at room temperature. The film exhibited a sharp absorption and the optical transparency in the wavelength range 750-1100 nm was more than 60 %. The oscillations in the transmission spectrum are caused by optical interference arising due to difference of refractive index of film with glass substrate and the interference of multiple reflections originated from film and substrate surfaces [14, 15].

Due to the existence of the interference pattern, which exhibits several maxima and minima as the wavelength increases, the anvelopes method of Swanepoel [12] was used to calculate the refractive index of the film. According to this method, the value of refractive index at determined wavelength can be calculated using the expression [12, 16-18]:

$$n = [N + (N^2 - n_s^2)^{1/2}]^{1/2} \tag{1}$$

$$N = 2n_s\left(\frac{T_{max} - T_{min}}{T_{max}T_{min}}\right) + \frac{n_s^2 - 1}{2} \tag{2}$$

where n_s=1.50 is the refractive index of the glass substrate, T_{max} and T_{min} are the values of the envelope at the wavelength in which the upper and lower envelopes and the experimental transmittance spectrum are target, respectively.

The computed values of the refractive index from room temperature transmission spectrum in the wavelength region of 500-1100 nm are plotted in Fig. 2(b). The refractive index is found to decrease with the increase in the wavelength of photon incident, and tends to be constant at higher wavelength.

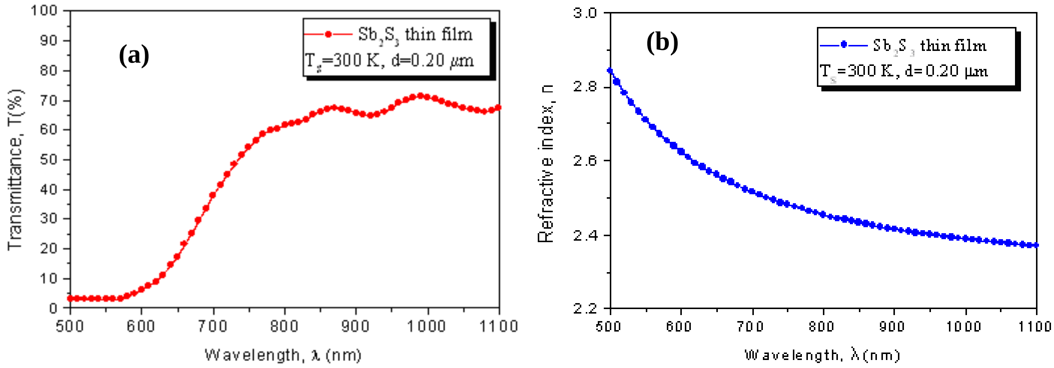

Fig. 2. (a) Transmission spectrum and (b) refractive index of Sb_2S_3 thin film deposited at 300 K.

The energy dependence of refractive index of amorphous materials can be fitted to the Wemple-DiDomenico single oscillator model [19, 20]. The model suggested that the relation between the refractive index and the single oscillator strength, below the fundamental absorption edge, could de described by the relation [21-24]:

$$n^2 - 1 = \frac{E_0 E_d}{E_0^2 - E^2} \tag{3}$$

where E_0 is the single oscillator energy, E_d is the dispersion energy and E=hν is the photon energy. By plotting $(n^2-1)^{-1}$ versus $(h\nu)^2$ and fitting the data to a straight line, E_0 and E_d can be determined from the intercept, (E_0/E_d) and the slope, $(E_0\ E_d)^{-1}$. The equation of straight line corresponding to least fit is $(n^2-1)^{-1} = 0.236 - 0.015(h\nu)^2$ (Fig. 3).

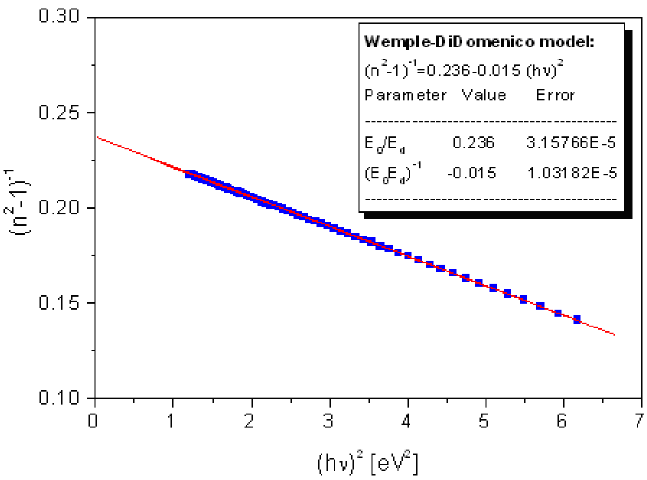

Fig. 3. Photon energy variation of refractive index dispersion factor $(n^2-1)^{-1}$ of Sb_2S_3 thin film.

The obtained values of E_0 and E_d for the investigated thin film are 3.96 eV and 16.79 eV, respectively. The single oscillator energy, E_0 is considered as an average energy gap to a good approximation, it varies is proportion to optical band gap energy E_g^{opt}: $E_0 \cong 2E_g^{opt}$ [25]. The E_g^{opt} value (1.98 eV) obtained from Wemple-DiDomenico model agree with those determined from spectral dependences of absorption coefficient for amorphous Sb_2S_3 thin film [8, 26-29].

4. CONCLUSIONS

In summary, Sb_2S_3 thin film has been deposited on a glass substrate by vacuum evaporation method and X-ray diffraction shows that it is an amorphous structure. Surface morphology studies of the thin film using AFM image reveals that the surface of the film is higher smooth. The refractive index of the Sb_2S_3 thin film was computed from transmission spectrum using Swanepoel's method. The optical band gap energy was calculated in terms of Wemple-DiDomenico single oscillator model. The band gap value was found to be 1.98 eV, which is in good agreement with the previously reported value of Sb_2S_3 thin film.

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Manuscript received: 30.04.2010
Accepted paper: 02.08.2010
Published online: 04.10.2010