

## INVESTIGATION OF STRUCTURAL AND OPTICAL PROPERTIES OF $Sb_2S_3$ THIN FILMS

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### Abstract

$Sb_2S_3$  thin films were obtained by evaporating the powder of  $Sb_2S_3$  compound onto glass substrates maintained at room temperature and at substrate temperature 423 K under vacuum pressure of ( $2 \times 10^{-5}$ ) torr. The composition of  $Sb_2S_3$  powder was determined by atomic absorption spectroscopy. The deposited films at room temperature were amorphous but the deposited films at 423K were polycrystalline structure. Optical parameters like absorption coefficient, energy gap, and refractive index were measured by the analysis of the experimental transmission spectrum over the wavelength range (200-1100) nm.

### Introduction

Antimony trisulphide ( $Sb_2S_3$ ) is considered as an interesting optical material in various optoelectronic device like television cameras<sup>[1]</sup>. The structure of thin films can be changed by preparation condition and preparation method<sup>[2]</sup>. Many researchers studied the characteristics of  $Sb_2S_3$  compound like Liker<sup>[3]</sup> who investigated the relation between rate of deposition and the structure of  $Sb_2S_3$  compound. In the present work, we studied the XRD patterns of  $Sb_2S_3$  thin films and transmission spectrum by Swanepoel method<sup>[4,5]</sup>. Swanepoel showed that the optical properties of a uniform thin film of thickness  $d$ , refractive index  $n$ , and absorption coefficient  $\alpha$ , which were deposited on a substrate with refractive index  $n_s$ , can be obtained from the transmission spectra by constructing two envelopes for the interference maxima  $T_M$ , and minima  $T_m$  in the transmittance spectra. The observed transmittance spectra were corrected relative to optically identical uncoated glass substrate. The optical energy gap and refractive index were measured by the transmission spectrum.

### Experimental

$Sb_2S_3$  thin films have been prepared onto glass substrates by thermal evaporation under vacuum ( $2 \times 10^{-5}$ ) torr of  $Sb_2S_3$  high purity polycrystalline powder (99.999% purity). The glass substrates were cleaned and were kept at room temperature and another at 423 K during the film deposition. The distance between the

molybdenum boat and the substrate was 10 cm. The deposition rate for all films was 0.5 nm/s. The thickness of the thin films was determined by Fizeau fringes method with equal thickness<sup>[2,6]</sup>, which was about (150) nm. The optical transmission spectrum of the deposited films was recorded using a Shimadzu and UV-visible recorder spectrometer UV-160. An Edward E306 A coating unit was used to prepare thin films.

### Results and Discussion

The composition of Sb and S of  $Sb_2S_3$  powder was measured by atomic absorption spectroscopy. It was nearly stoichiometric (44% Sb and 56 % S).

Fig.(1) showed that the X-ray diffraction patterns of  $Sb_2S_3$  powder and for thin films at R.T and at 423 K. It was clear that the prepared film at room temperature is amorphous and becomes polycrystalline with orthorhombic structure at 423 K which is due to the larger mobility of atoms to arrange themselves in large crystalline grains at higher substrate temperature with preferential orientation of crystallites along the (310) plane.

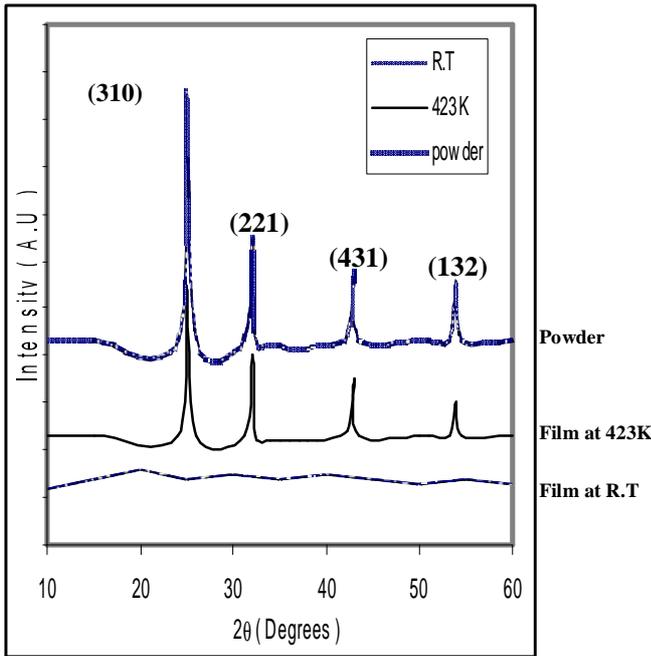


Fig. (1): XRD patterns of Sb<sub>2</sub>S<sub>3</sub>.

As shown in Fig. (1) the interplanar spacing  $d_{(hkl)}$  was calculated using the Bragg's equation.

$$d_{hkl} = n\lambda / (2 \sin\theta)$$

where  $\lambda$  is the X-ray wavelength,  $n$  is the spectrum order, and  $\theta$  is the diffraction angle. The calculated values of  $d_{hkl}$  for Sb<sub>2</sub>S<sub>3</sub> thin films at 423 K, are in good agreement with the standard values as shown in Table (1). The calculated lattice parameters were :

$$a = 11.4 \text{ \AA}, b = 11.22 \text{ \AA}, \text{ and } c = 4 \text{ \AA}.$$

Table (1)  
Comparison of experimental  $d_{hkl}$  with standard values for Sb<sub>2</sub>S<sub>3</sub> thin film.

(hkl)	2θ(deg.)	$d_{hkl}$ (Å°)		(I %)
		Exper.	Standard	
(310)	25.41	3.593	3.558	85.50
(221)	32.86	2.716	2.764	28.40
(431)	47.31	1.960	1.940	20.50
(132)	54.50	1.690	1.691	15.02

Fig.(2) shows the spectral behavior of the transmittance spectra for Sb<sub>2</sub>S<sub>3</sub> thin films deposited at room temperature and at substrate temperature (423)K at film thickness (150) nm. The value of substrate transmittance was found to be 93%. The dashed curves indicated the interference maxima,  $T_M$ , and minima,  $T_m$ . As shown from Fig. (2) the films have an average transmittance of 64 % over (750-1100) nm range .

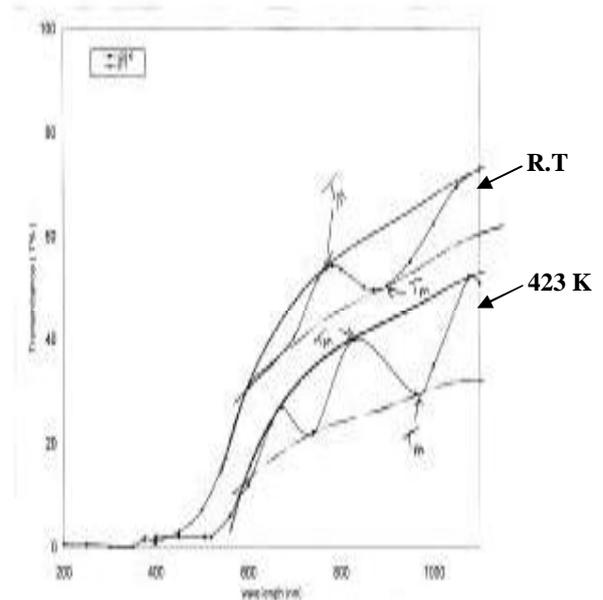


Fig.(2): Transmittance spectra of Sb<sub>2</sub>S<sub>3</sub> thin films as a function of wavelength.

The refractive index ( $n$ ) of a uniform thin film, for a determined wavelength, is given by

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

Where 
$$N = \left[ \frac{(1 + n_s^2)}{2} \right] + 2n_s \frac{(T_M - T_m)}{T_M * T_m}$$

Where  $n_s$  is the refractive index of the substrate and  $T_M$ ,  $T_m$  represents the maxima and minima peaks as shown in Fig. (2) respectively. From Fig. (2), the extrapolated envelope method has been employed to extract the refractive index,  $n$ , of the Sb<sub>2</sub>S<sub>3</sub> films by taking many points which locate on the extrapolated envelope. The refractive index was found to decrease with the increase of wavelength as shown in Fig. (3).

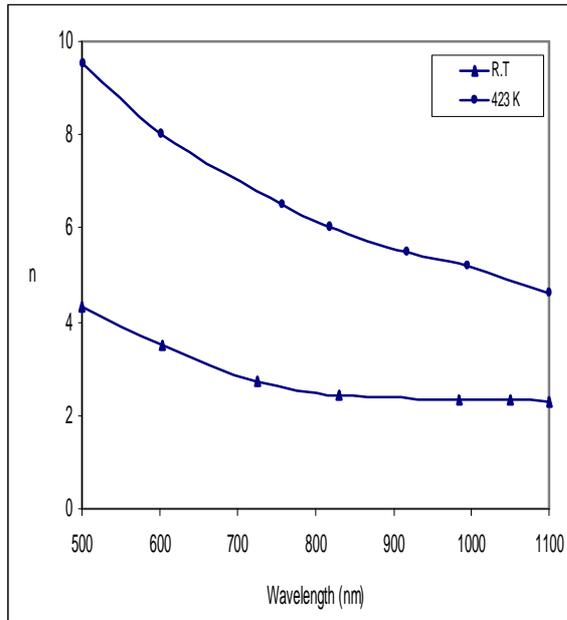


Fig.(3) : The refractive index of Sb<sub>2</sub>S<sub>3</sub> thin films.

Also, the optical energy gap was measured in the fundamental absorption edge by using the expression for the absorption coefficient, for allowed direct energy gap<sup>[7,8]</sup>, as

$$(\alpha hv) = A (hv - E_g)^{1/2} \dots\dots\dots (1)$$

Where  $h\nu$  is the photon energy,  $E_g$  represents the energy gap, and  $A$  is constant.

Fig.(4) shows the relation between  $(\alpha h\nu)^2$  against  $h\nu$ , from the figure, the energy gap was determined by the intercept of the linear part of the curve with X-axis and was found to be ( 2.4 and 2.0 ) eV at room temperature and at 423 K respectively with allowed direct transition. The decrease in energy gap at higher substrate temperature is due to the improved crystalline structure.

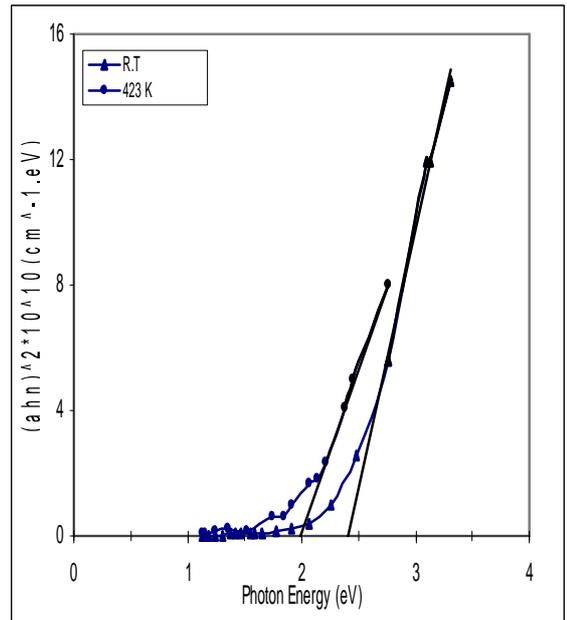


Fig. (4) : Plot of  $(\alpha h\nu)^2$  against  $h\nu$ .

**Conclusion**

Sb<sub>2</sub>S<sub>3</sub> powder exhibited good stoichiometry as analyzed by atomic absorption spectroscopy. It was clear that the film prepared at room temperature is amorphous and became polycrystalline with orthorhombic structure at 423 K. A lower transmittance is observed for such films with condition of substrate temperature (423)K at film thickness (150) nm. The optical energy gap was found to be (2.4 and 2.0) eV at room temperature and at 423 K respectively. The refractive index for thin films deposited at 423 K was higher than thin films deposited at R.T.

**Reference**

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#### الخلاصة

حصل على اغشية  $Sb_2S_3$  بواسطة تبخير مسحوق مركب  $Sb_2S_3$  على قواعد زجاجية عند درجة حرارة الغرفة وكذلك في درجة  $423\text{ K}$  وتحت ضغط ( $2 \times 10^{-5}$  torr). فحصت نسب مكونات المركب  $Sb_2S_3$  بواسطة تقنية مطياف الامتصاص الذري. وجد ان الاغشية المرسبة بدرجة حرارة الغرفة تكون عشوائية التركيب اما تلك المرسبه عند درجة حرارة  $423\text{ K}$  فهي ذات تركيب متعدد التبلور. قيست الكميات البصرية مثل معامل الامتصاص الكتلي  $\alpha$  وفجوة الطاقة  $E_g$  وكذلك معامل الانكسار  $n$  عن طريق دراسة طيف النفاذية ضمن مدى الاطوال الموجية  $(200-1100)\text{ nm}$ .