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Annealing Effect On Structural And Optical Properties Of Sb_2S_3 Thin Film

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Abstract. The effect of annealing on the structural and optical properties of Antimony trisulfide (Sb2S3) is investigated. Sb2S3 powder is vaporized on clean glass substrates at room temperature under high vacuum pressure to form thin films. The structural research was done with the aid of X-ray diffraction (XRD) and atomic force microscopy (AFM). The amorphous to the polycrystalline transformation of these thin films was shown by X-ray diffraction analysis after thermal annealing. These films' morphology is explained. The absorption coefficient and optical energy gap of the investigated films are calculated using transmission spectra. Both samples have strong absorption in the visible spectrum, according to UV-visible absorption spectra. The optical band gap is measured using as-deposited Sb2S3 thin films at room temperature and annealed Sb2S3 thin films at 473 and 573 K.

Keywords. (Sb_2S_3) Films, Annealing Effect, Thermal evaporation, Structural properties, Optical properties.

INTRODUCTION

Sb_2S_3 is a V2-VI3 layered semiconductor. In recent years chalcogenides thin films physical properties have gained increased attention due to their various applications in optoelectronic devices [1, 2], Sb2S3 has a band gap that varies between 1.8 and 2.5 eV depending on the preparation conditions [3,4] . This material has been used in various areas such as solar energy conversion, photoconductive target for vidicon type of television camera and thermoelectric cooling technologies [5, 6], Sb2S3 thin films with an approximate thickness of 1 μm can absorb almost 95% of the solar radiation[7] , Depending on the process involved and deposition temperature, Sb2S3 thin films can be amorphous or polycrystalline in structure. Many scientists have obtained the amorphous Sb2S3 thin films by various techniques, including chemical bath deposition [8], sol-gel method [9], vacuum evaporation method [10, 11].The aim of the this research is to examine the effect of thermal annealing on the structural and optical properties of Sb2S3 thin films prepared by thermal evaporation technique.

EXPERIMENTAL DETAILS

Sb2S3 in bulk form was prepared by melting stoichiometric amounts of the elements antimony Sb and sulfur S of 99.99% purity to yield the Sb2S3 crude ingot. The mixture was vacuum-packed in a quartz tube. the tube's temperature was increased slowly (100 C/h) to avoid any possibility of explosions because of the high vapor pressure of the sulfur, sustaining the melt at 650 C for 3 h will result in complete homogenization of the sample. The tube was then cooled at 80 C/h rate. Therefore, avoiding cracking due to thermal expansion of the melt on solidification. Grinding the initial ingot yields the crude material for vacuum thermal evaporation .Sb2S3 films were deposited on a glass substrate by thermal vacuum evaporation under an approximately ($4.5x10^{-5}$ mbar) vacuum at room temperature. by using the weighing method the thickness was (500 ∓ 10) nm, and the deposition rate of about

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(1∓0.1) nm/sec. using (Edwards-Unit 306) system. Optical transmission measurements were performed with (UV/Visible 1800 spectrophotometer). The crystal structure of these films was examined using the X-ray diffraction method. The (SHIMADZU Japan -XRD600) automated diffract meter was used to extract the (XRD) patterns, which were obtained using CuKα radiations (λ=1.54059) in the range of 2θ between 10° and 80°. Atomic force microscopy (AFM) measurements were used to determine the nanocrystalline topography, and grain size of the films (SPM model AA 3000 Angstrom Advanced Lns., USA).

RESULTS AND DISCUSSION

The X-ray diffraction patterns of Sb2S3 powder are seen in Figure 1. The prepared powder is polycrystalline with an orthorhombic structure and crystallites that preferential orientation along the (320) plane. The obtained result is in accordance with the ICDD standard card (00-042-1393).

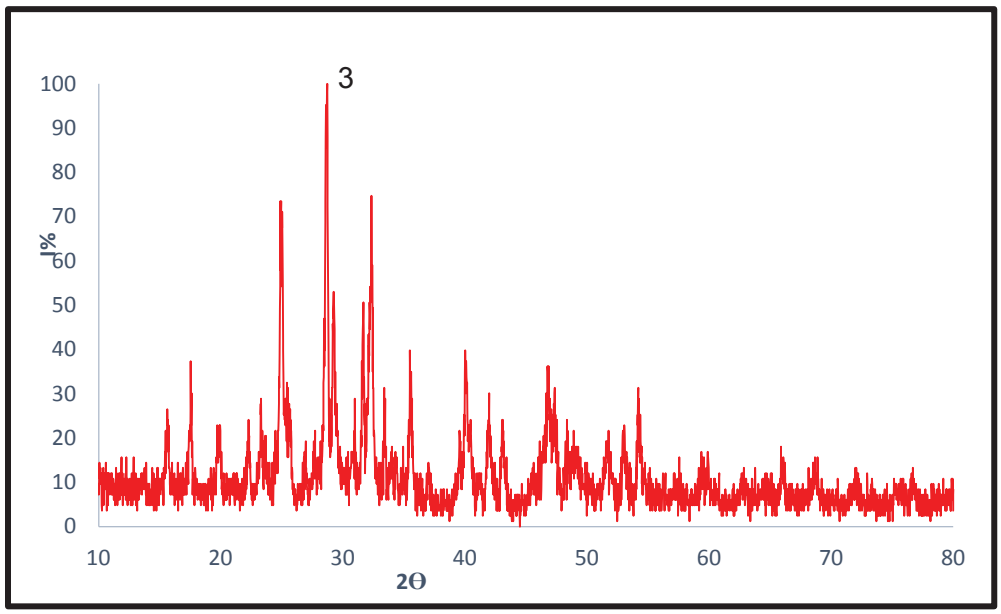

FIGURE 1. X-ray diffraction of the Sb2S3 powder

The X-ray diffraction (XRD) analysis shows that, at substrate temperature of 300 K , The deposited Sb_2S_3 films retain an amorphous structure Figure 2. Even after annealing at 473K the Sb2S3 thin films structure remains amorphous, the thin films show a polycrystalline structure after annealing at 573k. d(hkl) (interplanar spacing) was calculated with Bragg's equation [12] .

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

Where (θ) is the diffraction angle, (n) is an integer the order of the reflection, and (λ) is the wavelength of the X-ray beam. Calculated d_{hkl} values for Sb2S3 thin films at 573 K are consistent with the standard values as shown in Table (1). Films that have been annealed at this temperature are crystallized in the orthorhombic phase, with a preferential orientation along the (320) plane, according to the XRD pattern.

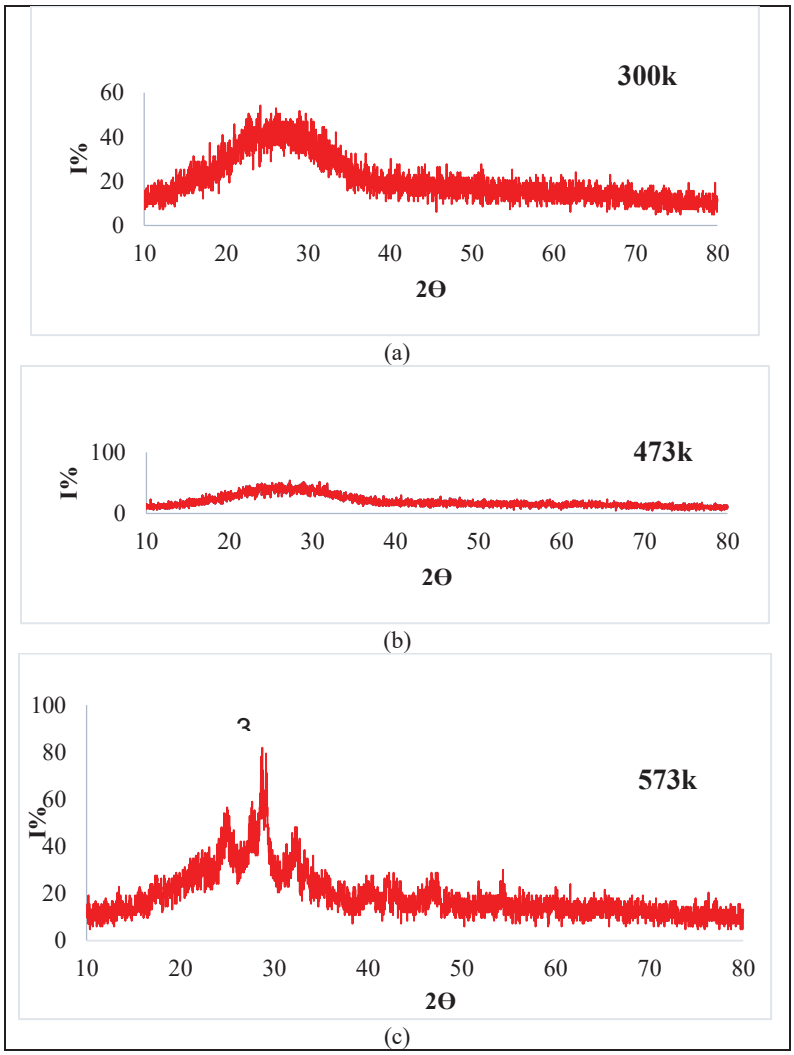

FIGURE 2. plot of X-ray diffraction of the Sb2S3 Thin film

TABLE 1. Experimental d_{hkl} with standard values for Sb_2S_3.

Sample	2θ Observed	2θ Stander	d(A°)Observed	d(A°)Standard	(hkl) Standard
Sb_2S_3 (powder)	28.6822	28.5118	3.10988	3.121000	320
	24.9985	24.8995	3.55917	3.575000	130
	32.3143	32.3632	2.76815	2.765000	221
Sb_2S_3 Thin film annealing at 573k	28.8648	28.5118	3.09063	3.121000	320
	24.8663	24.8995	3.57779	3.575000	130
	32.2507	32.3632	2.77346	2.765000	221

We have used Atomic Force Microscopy (AFM) to study the surface morphologies of the Sb2S3 films. Their surface morphologies are shown in Figure (1). The measured roughness, RMS roughness and grain size are provided in Table (2). It is understood from Table (2) that the size of the grains increases with annealing temperature. Because of the growth of smaller grains together to form larger grains which led to the enhancement of structural properties. The surface roughness root mean square values were estimated to be between 12.2 and 14.3 nm.

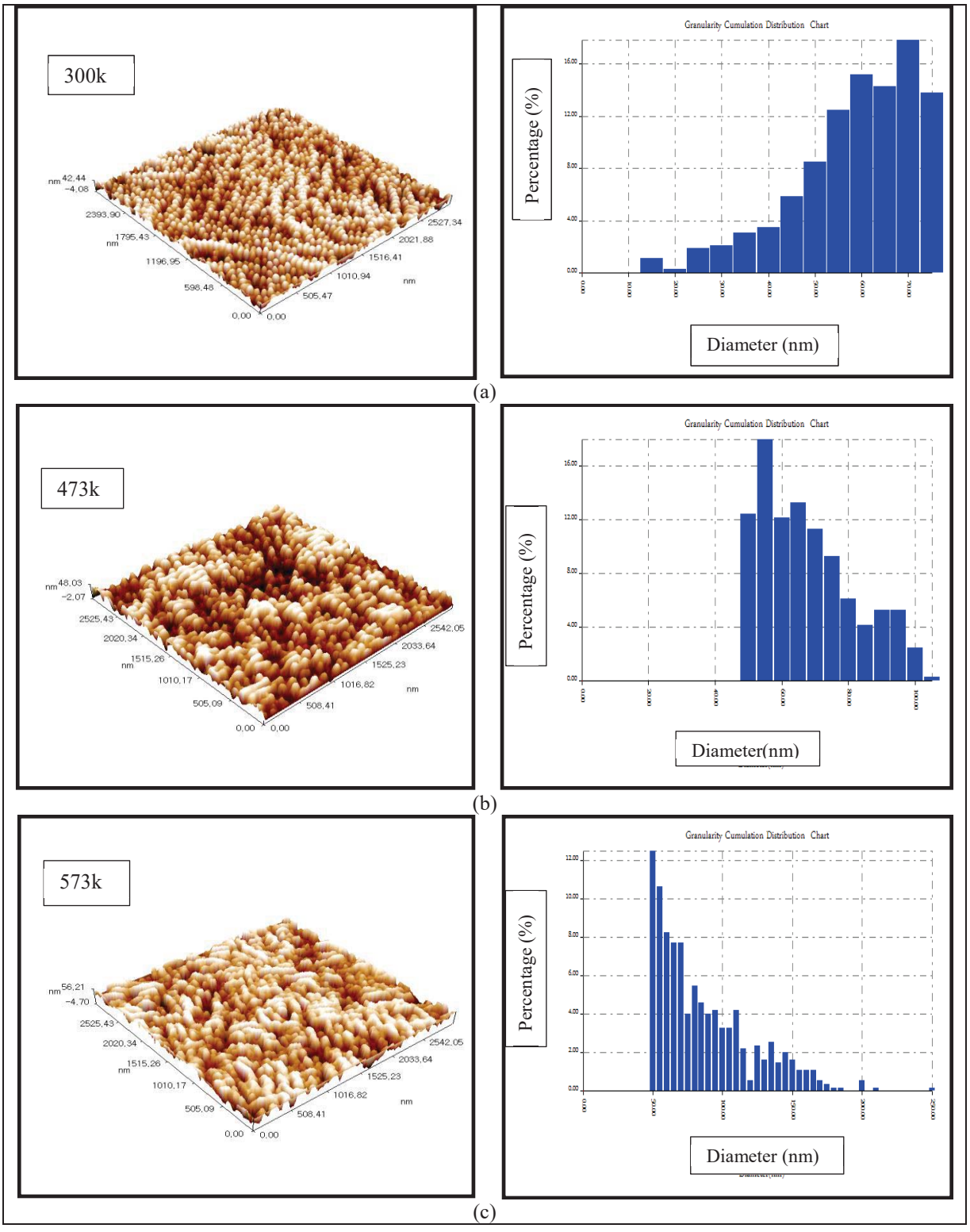

FIGURE 3. AFM images of Sb_2S_3 thin films

TABLE 2. AFM results for Sb2S3 thin films.

Samples	Avg. grain size (nm)	Roughness(nm)	r.m.s (nm)
300k	56.35	10.3	12.2
473k	65.54	11.6	13.5
573k	83.99	12	14.3

Band structure and energy gap comprehension and development of both amorphous and crystalline materials are done through optical absorption spectra analysis. The transmittance spectra were measured as a function of wavelength in the spectral region (300-1100) nm at 500 nm thickness for (Sb_2S_3) films at room temperature and for annealing at (473 and 573) K as presented in Figure (4). Figure (5) displays the presence of an absorption edge and shows that the optical absorption coefficient (α) is a function of photon wavelength. The optical absorption coefficient in the material is on the order of 10^4 cm^{-1}, indicating a direct and allowed band transition [13].

Transition's nature can be determined on the basis of absorption coefficient (α) dependence of on photon energy (hυ). For allowed direct transition, The energy gap (Eg) of the Sb_2S_3 thin films is calculated using the expression [14, 15]:

$$\alpha h\nu = A\,(h\nu - Eg)^{r} \qquad (2)$$

Where A is constant, α (cm^{-1}) is the absorption-coefficient, Eg (eV) is the energy gap , (hν)(eV) is the photon-energy. (r) is determined by the optical transition involved in the absorption process. The energy gap was obtained from the intersection of the photon energy axis by the straight line of the curve $(\alpha h\nu)^2$ versus (hν) plot as Shown in Figure(5). The optical band gaps as a function of temperature are shown and was found to be (2.0) eV at room temperature, it decreased from 2.1 eV at 473 K to 1.6 eV at 573 K with allowed direct transition. At higher temperature, The diminishing energy gap is due to the improved crystalline structure. the effect of increasing the temperature of annealing on the energy gap can be noted from the Table (3), reported values of Sb_2S_3 thin films prepared using various methods are in agreement with These values [15,16].

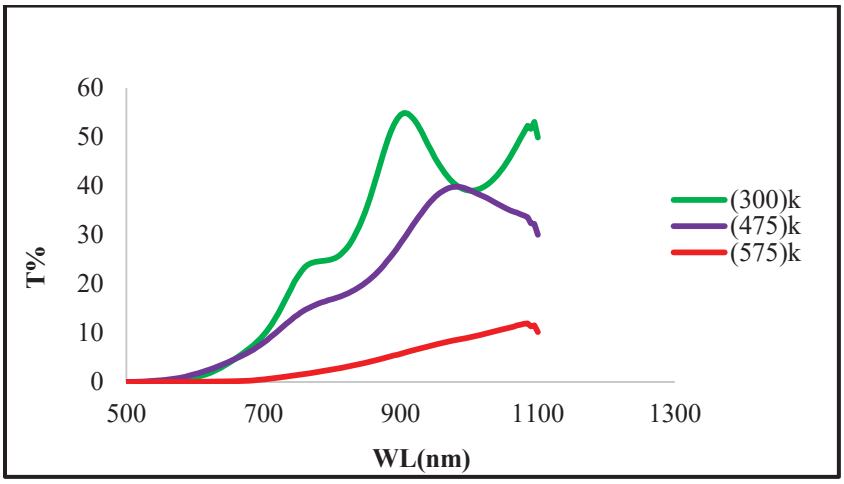

FIGURE 4. Optical transmittance versus wavelength for Sb2S3 thin film

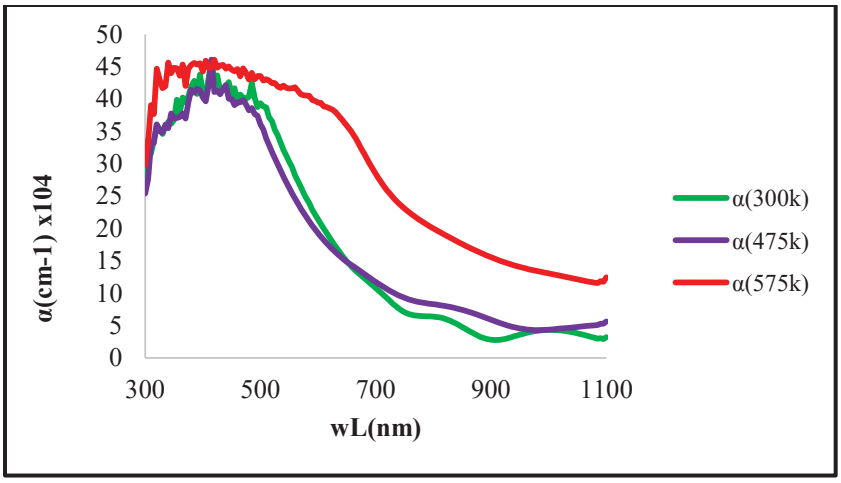

FIGURE 5. Optical absorption coefficient versus wavelength for Sb2S3 thin film.

TABLE 3. Band gap (Eg) of as-deposited and thermally treated.

Sample	Eg (eV)
300k	2.0
475k	2.1
575k	1.6

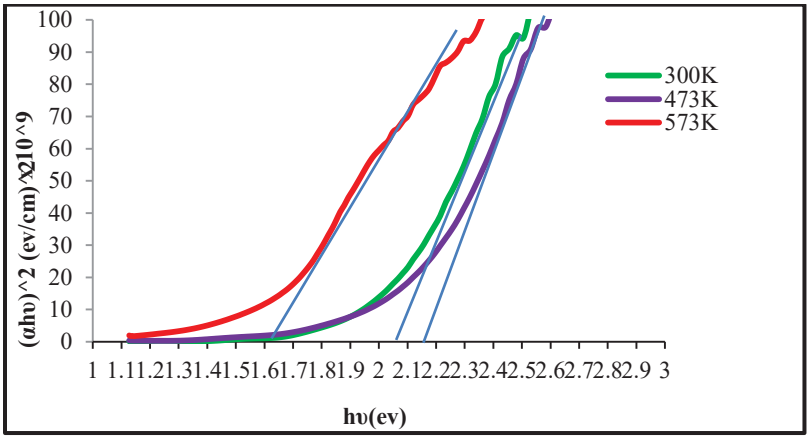

FIGURE 6. Plot of $(\alpha h\upsilon)^2$ against $(h\upsilon)$ for Sb2S3 thin film

CONCLUSION

Sb2S3 powder was prepared successfully. It was apparent that the thin film prepared at room temperature has an amorphous structure and alters to a polycrystalline with orthorhombic structure at 573 K. The absorption coefficients were determined to be between 10^4 and 10^5 cm^{-1}. At room temperature, the optical energy gap is (2.0) eV, and at (473,573) K, it is (2.1, 1.6) eV respectively. The characteristics recorded in this study suggest that Sb2S3 could be used as an absorber material in solar cells.

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