Investigation of the Structural and Optical Properties of Bismuth Telluride (Bi_2Te_3) Thin Films

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Abstract: In the preparation of Bismuth Telluride thin films are reported in the present work. Measurements of the structural and optical properties of Bi_2Te_3thin films were studied by X-ray diffraction, transmission (TEM) and scanning (SEM) electron microscope and electron diffraction techniques. Bi_2Te_3 thin films were "polycrystalline" Hexagonal form. The crystallite size was determine .The optical energy gap was evaluated. The study was carried out under vacuum., These properties has been reported to date. It was found from the optical properties studies that the type of transition of Bi_2Te_3 is an indirect transition.

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Key wards: Thermal evaporation, Structure , Bismuth Telluride – Thin Films

1. Introduction

Bismuth chalcogenides materials such as Bi_2Te_3 and Bi_2Se_3 comprise some of the best performing room temperature thermoelectric with a temperature-independent thermoelectric effect.[1] Nano structuring these materials to produce a layered super lattice structure of alternating Bi_2Te_3 and Bi_2Se_3 layers produces a device within which there is good electrical conductivity but perpendicular to which thermal conductivity is poor. [2]

Bismuth telluride compounds are usually obtained with directional solidification from melt or powder metallurgy processes. Materials produced with these methods have lower efficiency than single crystalline ones due to the random orientation of crystal grains, but their mechanical properties are superior and the sensitivity to structural defects and impurities is lower due to high optimal carrier concentration.

The required carrier concentration is obtained by choosing a nonstoichiometric composition, which is achieved by introducing excess bismuth or tellurium atoms to primary melt or by dopant impurities. Some possible dopants are halogens and group IV and V atoms. Due to the small band gap (0.16 eV) Bi_2Te_3 is partially degenerate and the corresponding Fermi-level should be close to the conduction band minimum at room temperature. The size of the band-gap means that Bi_2Te_3 has high intrinsic carrier concentration. [3]

Narrow-gap semiconductors have attracted considerable interest due to their wide application in infrared optoelectronics[4]. Bi_2Te_3 is a narrow gap semiconductor[5] . Belonging to the family of V-VI compounds of the general type Bi_2X_3 (X = Te, Se, S). Nevertheless some of the transport properties of Bi_2Te_3 have been scarcely reported, especially no detailed study of the electrical conductivity and Hall coefficient in a wide range of temperature has been performed[6-8].

The shape of the absorption edge in the semiconductor Bi_2Te_3 has been determined from transmission measurements on cleavage sections. The edge is of the form expected for indirect transitions, but an interpretation in terms of phonons characterized by a single energy is not applicable. A brief study of anisotropy effects is included. The energy gap at room temperature is close to 0.13 eV.[9,10]

2. Experimental and Measurement technique :

The preparation for structural and optical properties of Bismuth Telluride $Bi_2Te_3$with a purity of 99.999%, thin films are reported in the present work. Bi_2Te_3 thin films were grown by a vacuum thermal evaporation technique which deposited on a flat cleaned glass substrates for the structural properties and quartz substrates for the optical properties with a thermal evaporation method. The structural properties of Bi_2Te_3 samples of 170 nm , 235 nm, 275 nm and 342nm thicknesses, have been analyzed using X – ray Diffraction (Philips, PW 1700) in the degrees range of 10°– 100° , and thewavelength $\lambda_{CuK\alpha}$ = 1.5418 Å. Measurements of these samples were performed at the room temperature. The effect of thicknesses are studied. The optical properties of Bi_2Te_3 samples with 45 nm, 130 nm, 154 nm, 202 nm, 245 nm thicknesses, have been analyzed using a spectrophotometer (Jasco V570) in the wavelength range of 200–2500 nm.

3. Results and Discussion:

The Bi_2Te_3 powder Fig.1.and as-grown at room[1-3] temperature samples with a different thicknesses of 170nm , 235nm, 275nm and 342nm,

Fig.2.were investigated by X-ray diffraction "Bragg's Law", which describes the condition for constructive interference from successive crystallographic planes.

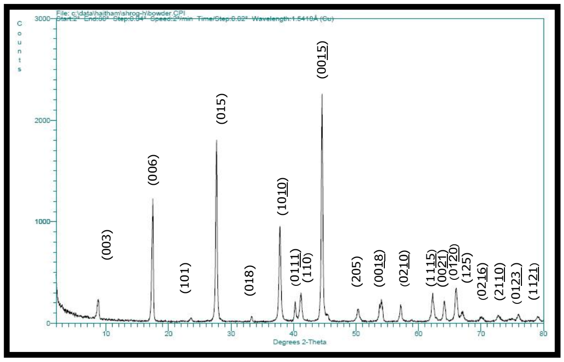

Fig. 1. X-ray diffraction of powder Bi_2Te_3.

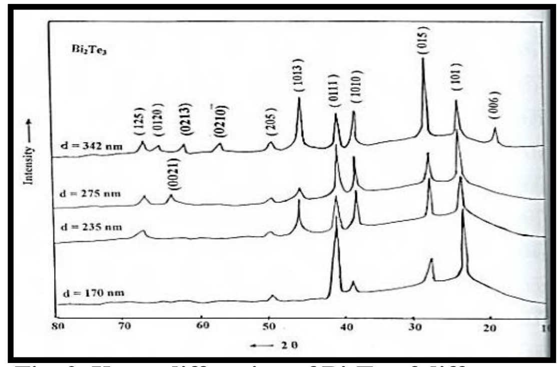

Fig. 2. X-ray diffraction of $Bi_2Te_3$of different thicknesses thin films.

The pattern indicated that both as – deposited and annealing films in vacuum at 443K for 1h Fig.3, were polycrystalline with a Hexagonal structure and the calculated lattice constant are a = 4.43Å , c = 30.55Å, highly oriented crystallographic growth ofBi_2Te_3 thin films of 342nm thickness as shown in Fig.3.

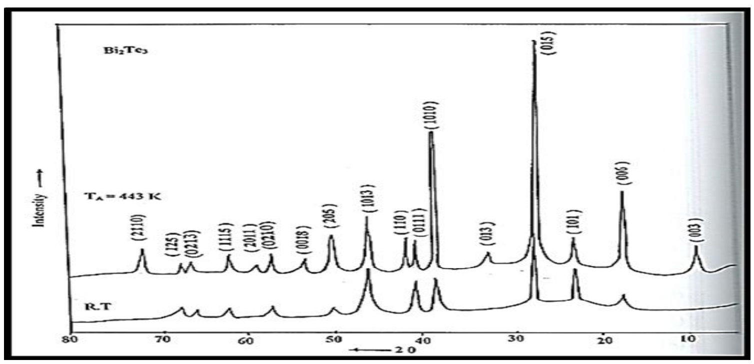

Fig. 3. X-ray diffraction of Bi_2Te_3 thin film of 342 nm thickness before and after annealing T= 443K, for 1h .

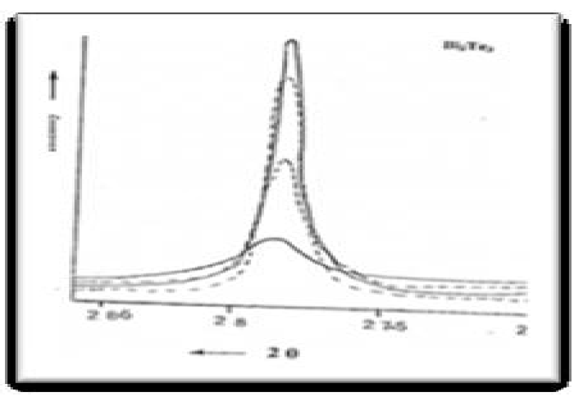

Fig.4. The full width of (015) peaks of a maximum intensity of different thicknesses.

The crystal size "Grain Size " D,Fig.4,was determined by inspecting its effect on the broadening of the X-ray line profiles by step scan, using Scherrer's formula.[11]

$$D = \frac{K\lambda}{\beta \cos\theta} \quad (1)$$

where: λ is the X-raywavelength, $\lambda_{CuK\alpha}$=1.5418 Å, K: is the shape factor "constant" =0.95, β:is the (015) full width at half maximum intensity= 9.89×10^{-3} and θ : is the scattering angle or the Bragg's angle . This leads to Bragg's law, which describes the condition for constructive interference from successive crystallographic planes, From the calculated the values of the grain size D, are listed in table [1].

Table [1]: The relation between the crystal size "Grain Size " D with the film thicknesses of Bi_2Te_3.

Film Thickness d (nm)	Grain Size D (nm)
170	60
235	110
275	150
342	160

This technique showed that the crystallite size increase as the film thickness increase. In addition, studies on the structural properties ofBi_2Te_3thin films of 60 nm thickness, involved both electron diffraction technique, scanning electron microscope (SEM) Fig.5and transmission electron microscope (TEM) Fig.6.were used to check the crystallinity of the films. These studies revealed that the crystallite size was relatively larger for annealed samples. Electron diffraction was used to obtain information about the structure of Bi_2Te_3 of 60 nm thickness. An electron diffraction pattern are shown in Fig.7.

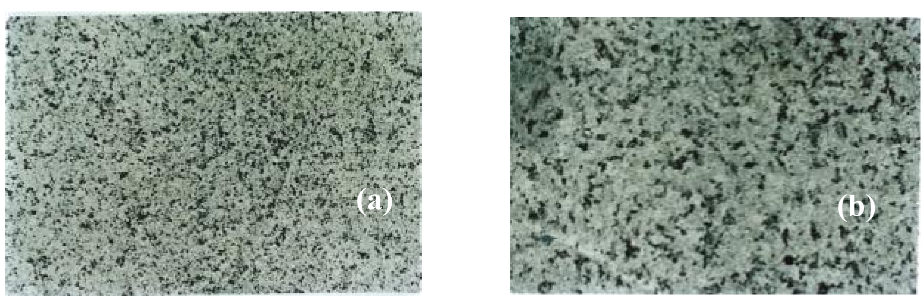

Fig. 5. SEM diffraction pattern of Bi_2Te_3 thin film indicating (a) before (b) after annealing.

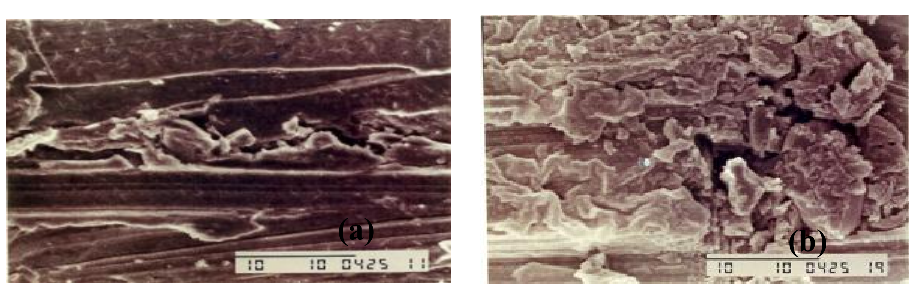

Fig. 6.TEM diffraction pattern of Bi_2Te_3 thin film indicating (a) before (b) after annealing.

Fig. 7. An electron diffraction pattern indicating (a) before (b) after annealing Bi_2Te_3thin films.

The results show that annealing does not change the polycrystalline, but its affect the size and shape of the coordination compound nanoparticles correspond with the size and shape of the samples, suggesting that the presented system increases the crystallite size.

The optical properties of Bi_2Te_3 samples, which have been analyzed using a spectrophotometer at room temperature from the Transmission and Reflection spectra of Bi_2Te_3thin films of various thicknesses are shown in Fig.8. The optical constants (refractive index n, absorption index k and absorption coefficient α) were determined for both n and k ,which are independent on the film thickness in the range of 105- 503 nm.

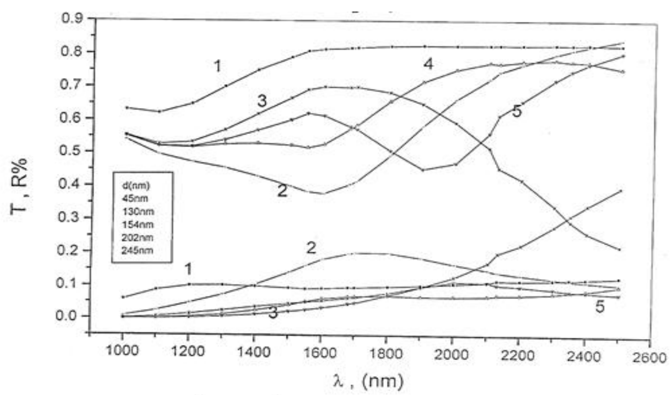

Fig. 8. Transmission and Reflection spectra of Bi_2Te_3thin films of various thicknesses.

From the analysis of spectral distribution of n and k, shown in Fig.9.

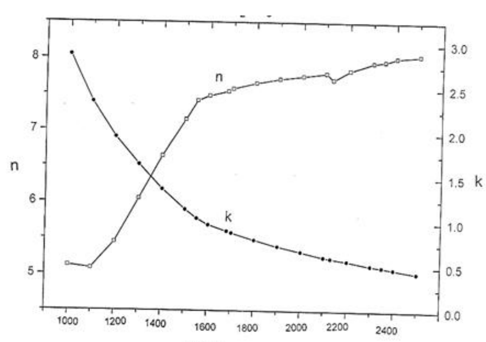

Fig.9. The analysis of Bi_2Te_3 spectral distribution of n and k.

It was found that the type of transition of Bi_2Te_3 is an indirect transition. The shape of the absorption edge in the semiconductor Bi_2Te_3. Fig.10, has been determined from transmission measurements on cleavage sections.

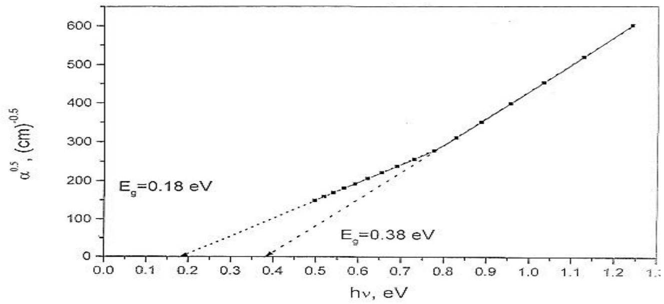

Fig.10.Relation of (αhν)$^{1/2}$Vshν plot for the Bi_2Te_3thin films.

The edge is of the form expected for indirect transitions, but an interpretation in terms of phonons characterized by a single energy is not applicable. It was found two edgeswith energy gap E_1^{ind}= 0.18 eV and the other one is E_2^{ind} = 0.38 eV.

4- conclusion:

The structural and optical properties of Bismuth Telluride Bi_2Te_3 were studied forBi_2Te_3 thin films of various thicknesses. These samples were investigated by X-ray diffraction, it's a polycrystalline thin films with " Hexagonal structure. Also the studies involved both electron diffraction technique , scanning electron microscope (SEM) , transmission electron microscope (TEM) and electron diffraction to check the crystallinity of the films. It was found from the optical properties studies that the type of transition of Bi_2Te_3 is an indirect transition.

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