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Dependence of Structure and Optical Characterization of (Bi_2Te_3) Films Prepared by Flash Evaporation on Annealing Temperatures

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ABSTRACT

In this study Bi_2Te_3 stoichiometry alloy was fabricated by using melting method in the electric furnce at temperature (580 ^{0}C for 6h). Thin films (Bi_2Te_3) were deposited by flash technique under vacuum 10^{-5} Torr . The thickness measured of films was 500nm .the influence of annealing temperature (100 -200) ^{0}C was studied structure and optical properties of Bi_2Te_3 thin films. Structural properties for thin films of Bi_2Te_3 were investigated by XRD and AFM analysis. The XRD analysis of alloy show that poly crystalline phase for Bi_2Te_3 stoichiometry while the films prepared were amorphous at room temperature and phase transition to polycrystalline under annealing with preffered orientation at (015) corresponding to(2θ =27.639) .FT-IR measured were studied for Bi_2Te_3 in range of (400-4000)cm^{-1} under annealing temperature and this measured show that decreasing of E_g with increasing annealing temperature ,this can be interpreted in term improved the crystal structure.

Keywords: Bi_2Te_3, XRD, AFM, FT-IR.

اعتماد الخاصية التركيبية والبصرية لغشاء (Bi_2Te_3) والمحضر بطريقة التبخر الوميضي على درجات حرارة تلدينة

الخلاصة

في هذا البحث فأن سبيكة البزموث-تيليريوم والتي تم حسابها وزنيا تم تحضيرها بطريقة الانصهار في فرن كهربائي وعند درجة حرارية تصل الى 580م^o ولمدة 6 ساعات .اما غشاء تلك السبيكة فقد تم تحضيـــــره بطريقة التبخير الوميضي وعند ضغط واطيء يصل الى 10^{-5} تور . الرئيسي والذي تمت دراسته في هذا البحث هو تأثير درجة حرارة التلدين علـــى الخواص التركيبية والبصرية للغشاء ضمن المـــدى (100-200)م^o .فبالنسبة للخواص التركيبية للغشـــاء فقد تمت دراستها باستخدام قياس نمط حيود الاشعة السينية وكذلك باستخدام قياس مجهر التركيب الدقيق لطبيعة سطح الغشاء .ان

تحليل حيود الاشعة السينيـــة اكد بـأن سبيكة البزموث-تيليريوم هـي فـي طورمتعدد التبلور امـا الغشـاء المحضر لنفس السبيكة فقد تبين انـــه في طور عشوائي عند درجة حرارة الغرفة ولكنه عند اجراء عملية تلـدين الغشـاء فأنـه يتحـول الـى الطـور متعدد التبلور .امـا خ واص الغشـاء البصـرية فقد تمت دراسـتها باستخدام قياس تحويلات فورير للاشعة تحت الحمـــراء حيث تبين ان فجوة الطاقة البصرية لمـادة الغشـاء تتناقص بازدياد درجة حرارة التلدين .

INTRODUCTION

Bismuth telluride based alloys have been an attractive thermoelectric material widely used in cooling devices and proposed for energy conversion applications around room temperature. These thermoelectric devices can be almost maintenance free and downsizing because of no moving parts. It is possible to extend the applications of thermoelectric devices for their feature of downsizing. Micro-thermoelectric cooling is a suitable technique for the local cooling of micro-sensors and devices as it can be microelectronically integrated [1]. Micro-thermoelectric generating can supply small electric power to low power devices and actually have been equipped into wrist watches [2].The primary candidate technology for downsizing of thermoelectric devices is to apply semiconductor-processing technologies including thin film fabrication. The key issue of micro-thermoelectric devices is how to fabricate thin films with high performance. The performance of thermoelectric materials depends on the thermoelectric figure-of-merit of the material, ZT[3], which is defined as

$$ZT=((S^2 *T)/(\rho*\kappa)) \quad \ldots.(1)$$

where S is the Seebeck coefficient, ρ is the electrical resistivity, κ is the thermal Conductivity, and T is the absolute temperature. The product (S^2/ρ) is defined as the power factor. The power factor should be maximized while the thermal conductivity should be reduced in order to achieve high efficiency thermoelectric materials. Recently, progress has been made in improving the figure-of-merit of thin film thermoelectric materials and a significant improvement in thermoelectric figure-of-merit may also be achieved by employing super lattice or quantum well structures [4]. There are presented many deposition techniques such as flash evaporated deposition [5], co-sputtering [6], pulsed laser deposition deposition [7], metal organic chemical vapor deposition (MOCVD) [8] and molecular beam epitaxy (MBE) [9].Thus, although there are many deposition techniques, sufficient results for the stage of practical use have not been achieved yet because of higher production cost for expensive equipments or inadequate thin film properties.

In these deposition methods, we employ the flash evaporated deposition method as the fabrication of bismuth telluride based alloys thin films. On the other hand, the performance of the thin films is relativity low without annealing. In fact, annealing processes are known to enhance the transport properties [10]. However, there are few reports of linking a structural feature by the effect of annealing and that of transport properties on the thin films fabricated by flash evaporated deposition. 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.[11]

Experimental and Measurement technique

Bi_2Te_3 alloy were prepared by addition Bi element with Te element with chemical ratio, into very clean quartz tube, this tube were closed under vacuum 10^{-2} Torr. The first quartz tube which contain Bi, Te and was heated up to (580^{o}C for 6 hours) with checking to be sure that there is complete mixing and homogeneity for each compound. The Bi_2Te_3 film of thicknesses (500 nm), were prepared using flash thermal evaporation under vacuum 10^{-5}mbarTorr using coating unit of type Edwards E 306 onto well-cleaned glass substrates at 27 ^{o}C. Bi_2Te_3 thin film formed by a flash thermal evaporation under a vacuum of 10^{-5} mbar. The stichometery of this compound was measured using Atomic absorption test where the weight of the alloy $Bi_2Te_3$was 5gm which 2.609gm for and 2.395gm for Te . Bi_2Te_3 thin films were grown by a flash thermal evaporation method. Our schematic of our experimental flash evaporated deposition set up is illustrated in Fig. 1. Which deposited on a flat cleaned glass substrates for the structural properties and quartz substrates for the optical properties with a flash thermal evaporation method. The structure of these powders and thin films were carried out using X-Ray Diffraction (XRD) of type Shimadzu XRD-6000, Japan, with wavelength (0.15425 nm) of CuKα1. The XRD measurements were in the angle range from 2θ(20^{o} - $60^{o)}$. The optical transmittance for this film was measured using FT-IR spectrophotometer Jasco (V-570) in the range of wave length (190 – 2500 nm). The effect of annealing temperatures are studied on the structural and optical properties of Bi_2Te_3 thin film. Where the samples of thin film of Bi_2Te_3 annealed at different temperatures (273- 473)k.

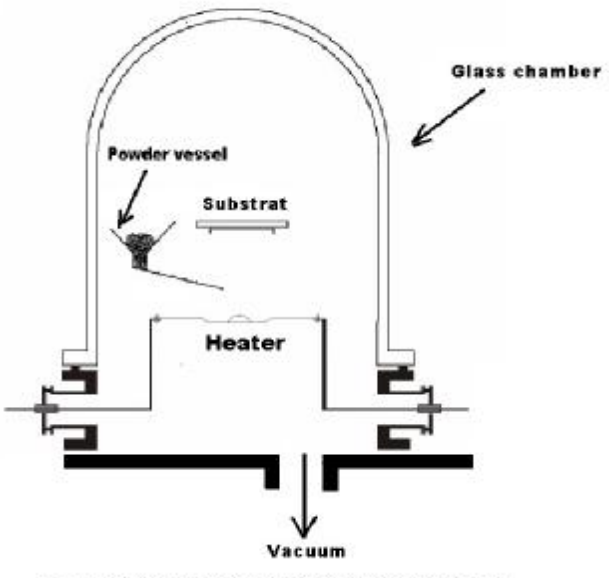

Figure (1).Schematic diagram of flash evaporated deposition

Results and discussion

The Atomic absorption measurement for the alloy of Bi_2Te_3 material have a nearly stoichiometry ratio because the ratio of elements of Bi_2Te_3 alloy was 53.51% : 46.39% respectively. Figure (1) shows the X-ray patterns of the Bi_2Te_3 alloy, from the figure (1) it is clear that alloy diffraction for this material have polycrystalline structure at room temperature [12] at thickness(500nm). Fig.2.show the XRD of Bi_2Te_3 thin film at different annealing temperatures(373 ,473)k, which describes the condition for constructive interference from successive crystallographic planes. The pattern indicated that annealing film in vacuum at (443k) for 1h was polycrystalline with a Hexagonal structure and the calculated lattice constant are a =4.43Å , c = 30.55Å, highly oriented crystallographic growth of Bi_2Te_3 thin films of 500 nm thickness as shown in figure(2). The crystal size "Grain Size " D, figure(2),was determined from Scherrer's formula.[13]

$$D=((k*\lambda)/(ß*\cos\theta)) \quad \ldots.(2)$$

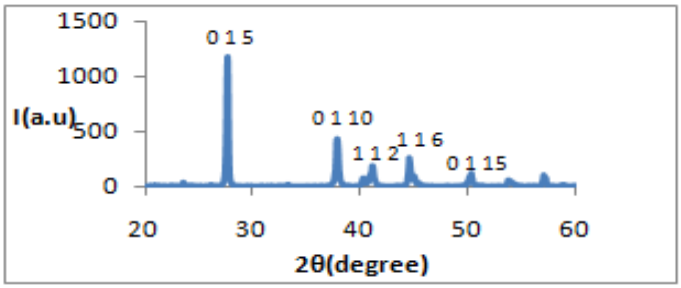

Figure (2) XRD of alloy of Bi_2Te_3

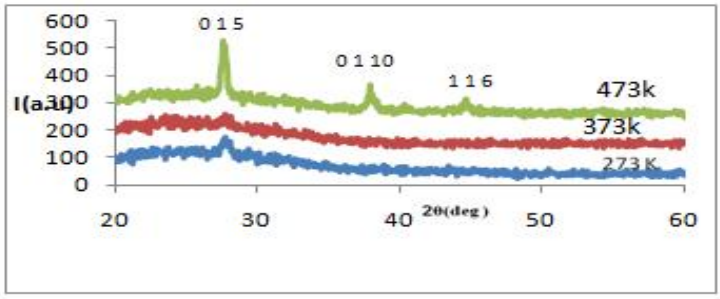

Figure (3) XRD of Bi_2Te_3 thin films annealed at different temperatures for 1h .

where: λ is the X-ray wavelength, λCuKα=0.15425 nm, K: is the shape factor "constant" =0.95, β:is the (015) full width at half maximum intensity= 9.89 $\times 10^{-3}$ 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 of Bi_2Te_3 at thicknesses 500 nm at different peakes intensities at (473k) .

d(A)	2θ Deg.	Int.	hkl	Grain size (A)	FWHM
3.2200	27.6630	100	015	176.9000	0.4625
2.3705	37.9254	34	1010	161.5000	0.5200

The as-grown thin film is not observed grains on this magnification of the micrograph and positional crystalanc , phases stand to growth . At annealing temperature of (473k), we confirm the grains where the size is approximately 178 nm. As annealing temperatures increase, the grain size of the thin films is enhanced. Finally, the grain size of the thin film reaches the same as the film thickness at annealing temperature of (473k). The as-grown thin film has weak and broad diffraction peaks that imply small grain size.. The diffraction peaks of the thin films are enhanced but the crystal orientation still remain random as annealing temperature increase. This clear in figure (3) which the AFM technique used to describe the effect of annealing temperature on morphology of the surface where the roughness of the surface is increase at thin film which annealing at (473K) a result of the diffiusion of volatile Bi.

The energy band gap of the films was calculated with the help of transmission spectra, using the Tauc [14] relation:

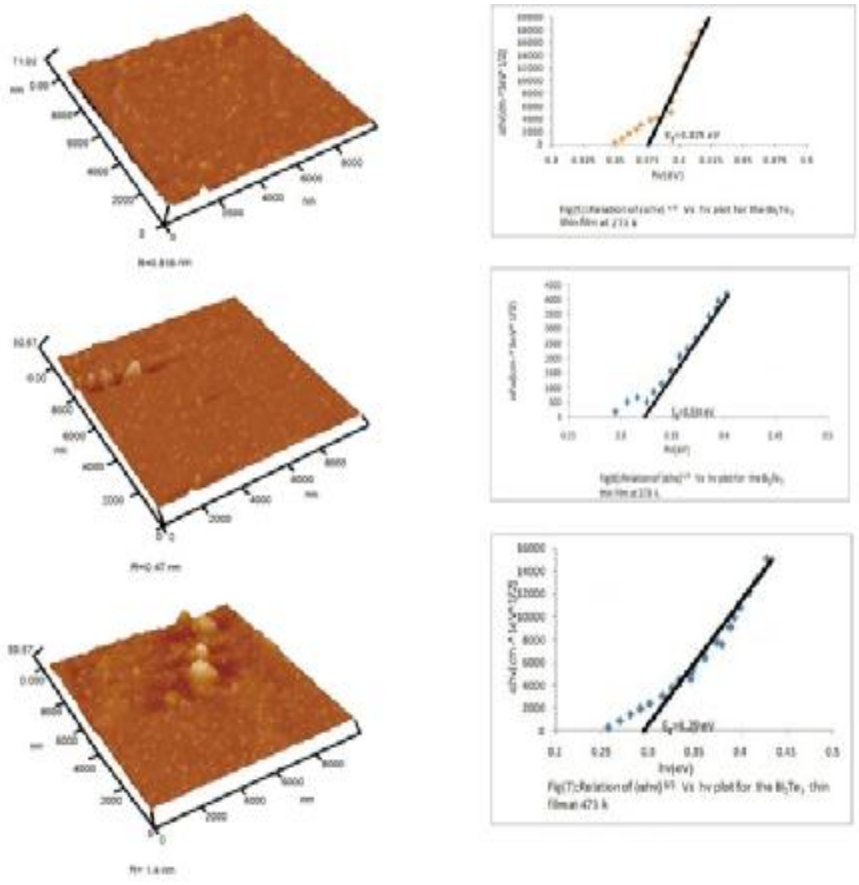

Figure (4).AFM images of Bi_2Te_3 film surface roughness.

$$\alpha h\nu = A(h\nu - Eg)^n \quad \ldots(3)$$

where

hν Photon energy
α Absorption coefficient
Eg Band gap
A Constant
n =½ for indirect band gap
n =2 for direct band gap.

Figure(4) , $(\alpha h\nu)^{1/2}$ Vs hν plot, the optical band gap energy has been estimated at 273k and by the same methods the optical band gap energy at 373k,473k of the films and given in Table (2). The possible transitions in theBi_2Te_3 thin films are indirect and allowed. It is observed from the table 2 the optical band gap shifts to a higher energy with increasing annealing temperature is due to the improvement of the crystallinity, thereby increasing the carrier concentration as determined from the Burstein–Moss effect[15].

Table (2): The relation between the optical energy gap and nealing temperatures of Bi_2Te_3thin film.

Annealing temperature (k)	Optical energy gap(eV)
273	0.375
373	0.334
473	0.29

CONCLUSIONS

The Bi_2Te_3 thin films grown by flash evaporation have been found to exhibit an amorphous nature. The annealing temperature of thin film leads to performance of structure to transform to hexagonal structure and the surface became rough. The possible optical transitions in these films are found to be indirect and allowed. The optical band gap decreases with an increase in annealing temperatures.

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