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SUBSTRATE TEMPERATURE EFFECT ON STRUCTURAL PROPERTIES OF Bi_2Te_3 THIN FILMS

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Structural properties of Bi_2Te_3 thin films, thermally evaporated on well-cleaned glass substrate at different substrate temperature, are reported here. X-ray diffraction was carried out for the structural characterization. XRD pattern of the films exhibits preferential orientation along the [0 1 5] *direction for the films of all the substrate temperature together with other supported planes* [2 0 5] *&* [1 1 0]. *All deposition conditions like thickness, deposition rate and pressure were maintained throughout the experiment. X-ray diffraction lines confirm that, the grown films are polycrystalline in nature with the hexagonal crystal structure. The effect of substrate temperature on these parameters have been investigated and reported in this paper. Various structural parameters such as lattice constants, grain size, micro strain, number of crystallites, stacking fault and dislocation density were calculated using X-ray diffraction analysis*

Keywords: *BISMUTH TELLURIDE THIN FILMS, X-RAY DIFFRACTION, STRUCTURAL PARAMETERS, DISLOCATION DENSITY, MICRO STRAIN, STACKING FAULT.*

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1. INTRODUCTION

The V_2-VI_3 (V = Bi, VI = Se, Te) binary compounds and their pseudo binary solid solutions are highly anisotropic and crystallize into homologous layered structure parallel to c-axis and are known to find applications ranging from photoconductive targets in TV cameras to IR spectroscopy [1, 2]. Among these Bi_2Te_3 is the most potential candidates for thermoelectric devices such as thermoelectric generators, thermocouples, thermo coolers and IR sensors with the best figure of merit near room temperature [3-6]. It also has applications in electronics, microelectronic, optoelectronic and electro-mechanical devices. It is a p-type semiconductor with a direct band gap of 0.21 eV and melting point 585 °C. The high ratio of the electrical conduction to the thermal conductivity makes bismuth telluride a good thermoelectric material [7-10]. There have been various studies on the optical and electrical properties of Bi_2Te_3 thin films. The dependency of thickness of film on structural properties were studied by Sathyamoorthy [11]. Here, the present authors report the structural variation in properties with the substrate temperature for a film thickness of 1000 Å.

2. EXPERIMENTAL DETAILS

Bi_2Te_3 compound was synthesized from its constituent elements of 99.999% purity. Bi and Te were sealed in quartz ampoule at a pressure of 10^{-5} torr in stoichiometric proportion. The ampoule was subjected to the alloy mixing furnace at the temperature of 620 °C. The temperature of the furnace was raised at the rate of 50 °C/hr and maintained for 24 hours. During this, the ampoule was continuously rocked and rotated for uniform mixing and homogeneity of the melt. Bi_2Te_3 thin films were deposited on the well-cleaned glass substrates held at different substrate temperature by thermal evaporation technique under the base vacuum of 10^{-6} torr. Here, the Bi_2Te_3 powder was taken from the ingot, in order to achieve better composition condition. The rate of deposition and the thickness of the film were measured to be 1 Å/s and 1000 Å respectively using the quartz crystal monitor.

The chemical composition of the ingot was obtained by EDAX(Philips ESEM). The X-ray diffraction patterns of the deposited Bi_2Te_3 thin films were recorded in the range of 20 - 70 degree with the help of Philips X-ray diffractometer using CuK_α radiation.

3. RESULT AND DISCUSSION

3.1 Compositional characterization

The typical EDAX, carried out for the synthesized ingot is shown in the Figure 1. The analysis confirms the stoichiometry of the synthesized compound with Bi and Te in the atomic percentage.

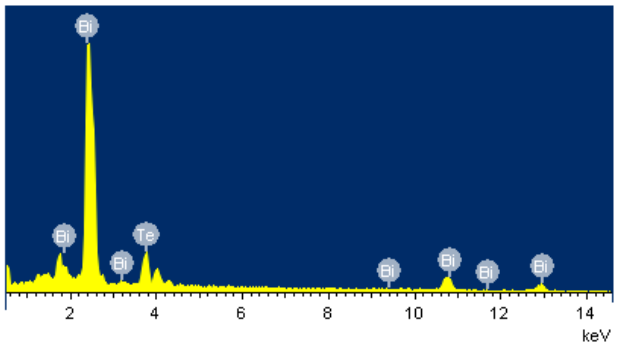

Fig. 1 *– EDAX of synthesized Bi_2Te_3 ingot*

3.2 Structural characterization

X-ray diffraction was carried out on evaporated Bi_2Te_3 thin films evaporated at different substrate temperatures and are presented in Figure 2. The thickness of the films was 1000 Å. They exhibited peaks at $2\theta = 22.54°$, 27.64°, 37.89°, 40.14° which corresponded to diffractions of (2 0 5), (0 1 5), (0 1 8) and (0 1 1) plane of hexagonal phases, respectively, indicating the polycrystalline nature of the films. The plane indices are obtained by comparing with the JCPDS # 020524 and #150863. The (0 1 5) hexagonal plane reflects Bi_2Te_3 phase present in the grown thin film.

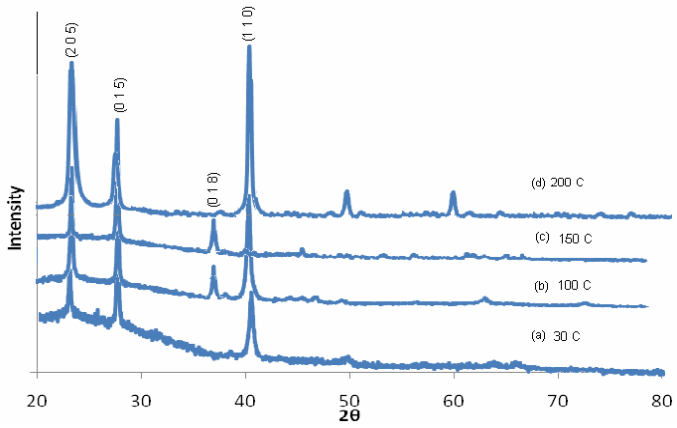

Fig. 2 *– XRD of Bi_2Te_3 thin film of substrate temperature (a)* 30 °C *(b)* 100 °C *(c)* 150 °C *(d)* 200 °C

The lattice parameter 'a' and 'c' are determined by using the relation for hexagonal crystal structure for the diffraction plane **(1 1 0)** and found to be a = 4.384 Å and c = 30.424 Å which are close to the reported values **[11, 12]**. The various structural parameters for Bi_2Te_3 thin films are calculated using the relevant formula **[11, 13, 14]** and are represented in Table 1.

Microstrain (ε):
$$\varepsilon = \frac{\beta_{2\theta}\cos\theta}{4}$$

Estimation of number of crystallites:
$$N = \frac{t}{D^3}$$

Dislocation density:
$$\rho = \frac{15\varepsilon}{aD}$$

Stacking fault:
$$3\alpha + 3\beta = \frac{\beta_{2\theta}\pi^2 c^2}{360ld^2\tan\theta} \quad \text{(for even } l\text{)}$$
$$3\alpha + \beta = \frac{\beta_{2\theta}\pi^2 c^2}{360ld^2\tan\theta} \quad \text{(for odd } l\text{)}$$

Where, $\beta_{2\theta}$ is the full width at half maximum, λ is the wavelength of CuKα radiation (1.54 Å), D is the mean crystallite size, t is the thickness of the film, ε is the microstrain, α is the deformation fault probability and β is the growth fault probability.

The grain size, micro strain, dislocation density and No. of crystallite of the deposited film at various substrate temperature was shown in Figure 3a, 3b, 3c, 3d respectively. As shown in Figure 3a, the grain size rapidly increases with the temperature upto 100 °C. No major change have been seen between 100 °C to 150 °C where as it again decreases with the increasing temperature. The larger grain size within this temperature range indicates the formation of good quality films.

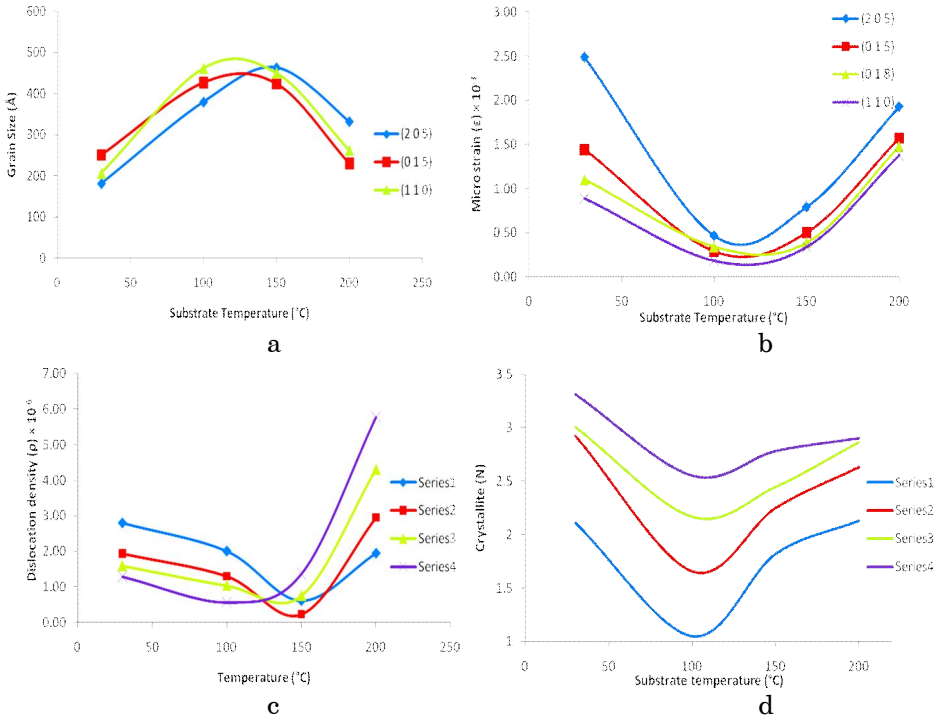

Fig. 3 *– Variation of (a) grain size (b) micro strain (c) dislocation density (d) No. of crystallite with substrate temperature*

Table 1 *– Structural parameters of thermally evaporated Bi_2Te_3 thin film at various substrate temperatures*

Subs. Temp. (°C)	*h k l*	*D* (Å)	$\varepsilon 10^{-3}$	$N{\cdot}10^{16}$ (cm^{-3})	$\rho 10^{-6}$(cm^{-2})	α	β
30	2 0 5 0 1 5 0 1 8 1 1 0	181.00 251.70 236.22 206.57	2.49 1.44 1.10 0.89	2.11 2.92 3.01 3.31	8.40 0.194 0.160 0.130	0.10812	– 0.10097
100	2 0 5 0 1 5 0 1 8 1 1 0	380.20 426.79 448.36 462.01	0.464 0.285 0.338 0.183	1.05 1.66 2.17 2.55	2.01 7.60 0.124 5.73	0.09793	– 0.08078
150	2 0 5 0 1 5 0 1 8 1 1 0	464.21 424.40 438.67 450.84	0.792 0.500 0.385 0.340	1.82 2.25 2.45 2.78	6.15 2.33 7.57 0.137	0.06782	– 0.04400
200	2 0 5 0 1 5 0 1 8 1 1 0	332.19 230.48 245.25 262.52	0.953 1.57 1.48 1.38	2.13 2.63 2.87 2.90	0.195 0.295 0.430 0.577	0.15142	– 0.12761

It is observed from Figure 3b, c and d that the micro strain, dislocation density and number of crystallite decrease up to 100 °C and then become steady up to 150 °C. These parameters again increase as the substrate temperature is raised further. The initialization of crystalline grains with considerable size was observed at 100 °C substrate temperature, as evident from Figure 2 and 3a. The maximum grain size was obtained for the substrate temperature between 110 °C and 150 °C. The structural properties depend upon arrangement of the evaporated atoms or molecules arriving on the substrate surface which possess larger kinetic energy at higher substrate temperatures. The appropriate substrate temperature gives large surface mobility and provides optimum diffusion distance of the evaporated atoms.

4. CONCLUSION

Bi_2Te_3 compound was synthesized from its constituent elements in a stoichiometric proportion and the maximum grain size 464.21 Å was obtained at 150 °C substrate temperature. Minimum micro strain 0.285 as well as dislocation density 0.124 were obtained for (0 1 8) plane at 100 °C. Whereas, the deformation fault probability α was reported 0.06782, higher than the growth fault probability β, − 0.04400, which indicate the lowest stacking fault probability at the substrate temperature of 150 °C. Thus, 100 °C to 150 °C is the optimum range of substrate temperature for the growth of high quality Bi_2Te_3 thin films using evaporation technique.

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