Optical Properties of Thin Film of $Bi_2Te_{3-X}Se_X$ (X=0.1&0.5) Compounds

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Abstract **–The best quality single crystal of $Bi_2Te_{3-X}Se_X$(X=0.1&0.5) was grown by using Bridgman technique with the freezing interface temperature gradient of 60˚C/cm and growth velocity 0.5 cm/h. Later on, the thin films of $Bi_2Te_{3-X}Se_X$(X=0.1&0.5) were grown at room temperature on the NaCl crystal substrate under pressure of 10^{-4}Pa by thermal evaporation technique. The room temperature deposited films of $Bi_2Te_{3-X}Se_X$(X=0.1&0.5) of various thicknesses were obtained. The optical absorption was measured in the wave number range 510 $cm^{-1}$to 4000 cm^{-1}. The optical energy gaps evaluated from these data were found to be inverse functions of the square of thickness, particularly for thicknesses about 2000 Å or less. This dependence is explained in terms of quantum size effect. For thicker films, the band gap is found to be independent of film thickness and approaches to the bulk value. The results are discussed in the view of the quantum size effect and reported in detail.**

Keyword: $Bi_2Te_{3-X}Se_X$, optical band-gap, Quantum size effect, Thermal Evaporation, FTIR

I. INTRODUCTION

Apart from the intensive research still going on the primitive elemental semiconductors at present much more attention is being paid to compound semiconductors, viz. binary, ternary and quaternary. Among the binary compound the group III-V semiconducting compounds have been receiving considerable attention due to their important in general electronic properties in the form of single crystals or thin films or both at a time. Fabrication of miniaturized and integrated thermoelectric devices using thin film techniques is highly required for the practical application. However, this mixed crystal material shows an important disadvantage that its material parameter changes with time. This is also a major remaining challenge for the application of III – V semiconductors in optoelectronic devices operating in the IR region. The III – V semiconductor structure have been investigated as an alternative for LWIR photo detectors[1-2].

Chalcogenidescompound of Bi,Sb,Te,Se have been widely used as the thermoelectric materials because of their relatively high conversion efficiency near room temperature. Those materials are narrow band gap semiconductors with a layered structure n-type of thermoelectric bismuth telluride thin films have been prepared and their characteristic properties were investigated according to the deposition temperature and post annealing process[3,4].

P-type material ternary $(Bi_{1-x}Sb_x)_2Te_3$(x=0.75) alloy are utilized in commercial thermoelectric modules. Therefore, researches on Bi-Sb-Te alloy in bulk form have been carried out [5-11]. Several works on the preparation and characterization of thin films have also been reported. The thin films were elaborated by a variety of deposition techniques, such as flash evaporation [12,13], ion beam sputtering [14], MOCVDtechniques [15],and molecular beam epitaxy[16]. The optical measurement constitutes the most important means of determining the band structure of semiconductors. For absorption studies, photons of selected wavelengths are directed at the samples and their relative transmission or absorption is measured.

In this paper $Bi_2Te_{3-X}Se_X$(X=0.1&0.5) single crystal were grown using Bridgman Technique and then films were prepared by thermal evaporation.

The thickness dependence of band gap of $Bi_2Te_{3-X}Se_X$(X=0.1&0.5) semiconductor, has been one of the main aims of the present study. The evaluation of the fundamental band gap variation with thickness $Bi_2Te_{3-X}Se_X$ (X=0.1&0.5) are discussed in view of quantum size effect.

II. EXPERIMENTAL DETAIL

Bi,Se,Te of 5N purity were weighted to stoichiometric proportions, up to a 10 microgram accuracy using semi micro balance and sealed under a vacuum of 10^{-4} torr in a quartz ampoule. The ampoule was kept horizontally in an alloy mixing furnace at a temperature of about 650°C for 48 hr. Then the ampoule was rocked and rotated for proper mixing and reaction .The ingot was then cooled to room temperature over a period of 24 hr at a rate of 200C/hr. The ingot was then subjected to zone levelling for homogenisation. Single crystal $Bi_2Te_{3-X}Se_X$(x=0.1, 0.5) were grown by Bridgman method with a temperature gradient of 600C/cm and a growth rate of 0.5cm/h, then the small chips of $Bi_2Te_{3-X}Se_X$(x=0.1, 0.5) were taken to prepare thin films of various thickness using thin film vacuum coating unit .The thin films were grown on a (001) face of NaCl substrate using the thermal evaporation technique at room temperature. An FTIR spectrophotometer was used for IR spectra. The optical absorption was measured in the wave number range 500 cm^{-1} to 4000cm^{-1}. The band gap has been evaluated from this data which was found to be dependent on the film thickness.

III. RESULT AND DISCUSSION

The plot of $(\alpha h\nu)^2$ versus hν were used to evaluate the optical band gap, where α = absorption coefficient and hν= photon energy. The plots are shown in Figure -1 for thin film of$Bi_2Te_{2.5}$:$Se_{0.5}$of thickness 1000Å. The plot is observed to be straight line in the region of high absorption side of the curves. The extrapolation of this linear part to the zero of abscissa has also been shown in the Figure-1, yielding the band gapvalue [17-18]. The thickness dependence energy gap has been shown in the table 1.

Such film thickness dependence of band gap has been explained in terms of quantum size effect and dislocation density [17-19]. In semimetals and semiconductors, the quantum size effect appears when the film thickness is comparable with or less than the mean free path or de Broglie wavelength of the carriers. Because of the small thickness of the films, the transverse component of the quasi momentum of carriers is quantized and it assumes discrete values along the thickness dimension. The energy spectrum represents a system of the discrete level with the separation between them given by the uncertainty principle. Due to this quantization, the bottom of the conduction band and the top of the valence band are separated by an additional amount ΔE [20].

In the thin films specimens, provided smearing of energy levels by temperature and diffuse scattering of the carrier at the film interface are not significant, this shift will increase the band gap and affect the optical behaviour of semiconductor thin films. The absorption is reduced in thin films as compared with that in the bulk. ΔE is givenby

$$\Delta E = \frac{h^2}{8m^* t^2} \qquad (1)$$

Here
m* = effective mass of charge carriers.
t = thickness of the films, h = Planck's constant.
ΔE = K.E contribution due to motion normal to the film plane.

The plots of Eg verses $1/t^2$ for $Bi_2Te_{2.5}$:$Se_{0.5}$ films given in Figure - 2 are in good agreement with the above relation and imply the quantum size effect operation in the thin films of $Bi_2Te_{2.5}$:$Se_{0.5}$ Compound.

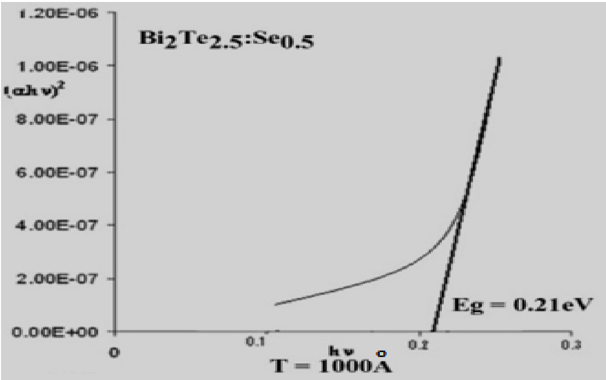

Figure – 1: The plot of $(\alpha h\nu)^2$ versus hν for $Bi_2Te_{2.5}$:$Se_{0.5}$ thin film.

Sample	**Thickness Å**	**Energy gap (eV)**
$Bi_2Te_{2.9}$:$Se_{0.1}$	1000	0.16
	1300	0.15
	1600	0.13
	2200	0.11
$Bi_2Te_{2.5}$:$Se_{0.5}$	1000	0.21
	1400	0.19
	1750	0.17
	1900	0.16

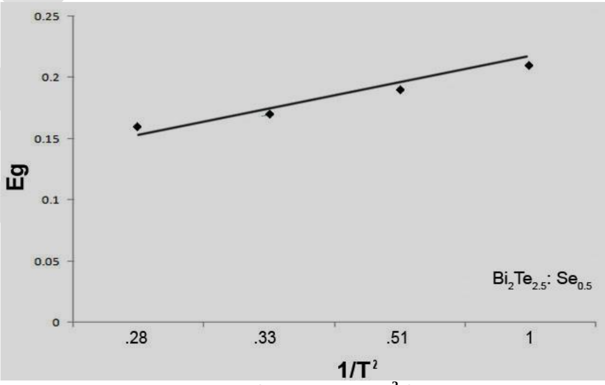

Figure – 2: The plot of Eg versus $1\backslash T^2$ for $Bi_2Te_{2.5}$:$Se_{0.5}$

IV. CONCLUSION

The optical, band gap of the thin films has been found to vary as Inverse Square of film thickness. The variation complies with the quantum size effect expected to dominate the carrier transport in the films.

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