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Optical bandgap of $Sb_{0.2}Bi_{1.8}Te_3$ thin films

P. H. SONI
Department of Physics, Faculty of Science, The M.S. University of Baroda, Vadodara 390 002, India

S. R. BHAVSAR
Department of Physics, C.U. Shah Polytechnic College, Surendranagar, India

C. F. DESAI
Department of Physics, Faculty of Science, The M.S. University of Baroda, Vadodara 390 002, India
E-mail: cfdesai@msn.com

$Sb_{0.2}Bi_{1.8}Te_3$ Thin Films were grown using the thermal evaporation technique on a (001) face of NaCl crystal as a substrate at room temperature. The optical absorption was measured in the wave number range 500 cm^{-1} to 4000 cm^{-1}. From the optical absorption data the bandgap has been evaluated and studied as a function of the film thickness and deposition temperature. The data indicate absorption through direct interband transition with a bandgap around 0.21 eV. The detailed results are reported.

1. Introduction

The V_2-VI_3 ($V_2 =$ Bi, Sb; $VI_3 =$ Se, Te) binary compound 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 T.V. cameras to I.R. Spectroscopy [1, 2]. Among these, Bi_2Te_3 is the most potential material for thermoelectric devices such as thermoelectric generators, thermocouples, thermo coolers and I.R. Sensors with the best figure of merit near room temperature [3–7]. It also finds applications in electronic, microelectronic, optoelectronic and electromechanical devices [2, 8]. Its melting point is 573°C and is a p-type semiconductors. There have been various studies on the bulk and thin film characteristics of Bi_2Te_3 including optical and electrical properties [9–12]. The authors have reported electrical resistivity of thin films of $Sb_{0.2}Bi_{1.8}Te_3$ [13]. However, there is no report on the bandgap study of $Sb_{0.2}Bi_{1.8}Te_3$ thin films. We hereby report the thickness dependence of optical band gap of $Sb_{0.2}Bi_{1.8}Te_3$ thin films.

2. Experimental

The material was synthesized using stoichiometric mixtures of the respective elements of 5N purity. The vacuum pressure used to seal the quartz ampoules containing the charge was of the order of 10^{-5} Pa. The sealed ampoule was kept in an alloy mixing furnace, providing rotation and rocking of the charge at the 623°C, i.e., 50°C above the melting point. After 48 hours of mixing, the molten charge was slowly cooled to room temperature over a period of two days. Thin films of $Sb_{0.2}Bi_{1.8}Te_3$ were prepared on the (001) face of NaCl crystal as the substrate using thermal evaporation method under a pressure of 10^{-5} Pa at room temperature, i.e., 313 K. The films were deposited at room temperature. The thickness of the film was measured by Tolansky's [14] multiple beam interferometric method. For optical study, a FTIR spectrophotometer (Bomem, Canada) was used.

3. Results and discussion

The optical absorption was measured in the wave number range 500 cm^{-1} to 4000 cm^{-1}. The absorption coefficient was calculated as a function of photon energy from absorbance versus wavelength curve. The plots of $(\alpha h\nu)^2$ versus $h\nu$ were used to evaluate the optical gaps. A typical plot is shown in Fig. 1 for a film of thickness 1900 Å obtained at 313 K. It can be seen that the plot is linear in the region of strong absorption near the fundamental absorption edge. Thus, the absorption takes place through direct transition. The band gap obtained by extrapolating the linear part to the zero of the ordinate is also indicated in the figure. The band gaps E_g were evaluated in this way for films of different thicknesses t. The band gap variation with film thickness follows the relation:

$$E_z = \frac{\eta^2\pi^2}{2m^*}\frac{1}{t^2}$$

where m^* is the effective mass of the charge carrier, t is the thickness of the film and E_z is the kinetic energy contribution due to motion normal to the film plane. Accordingly, the plot of E_z vs. $1/t^2$ is found to be linear (Fig. 2). This variation can be explained in terms of quantum size effect. This is usually defined as the

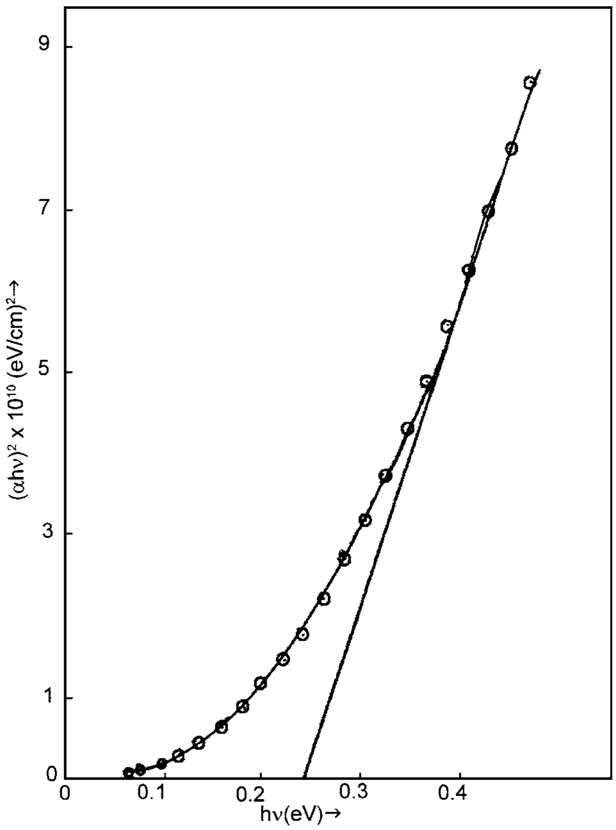

Figure 1 Plot of $(\alpha h\nu)^2$ versus hν (film thickness = 1900 Å).

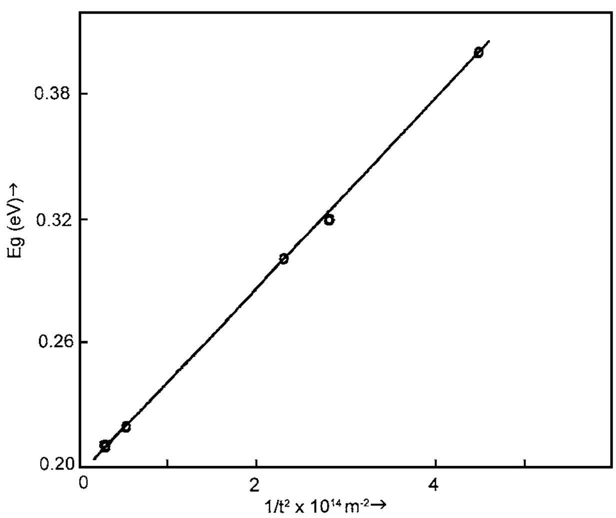

Figure 2 Plot of E_z versus $1/t^2$.

dependence of certain physical properties of a solid on its characteristic geometric dimensions when these dimensions become comparable to the de Broglie wavelength of the charge carriers [15, 16]. Because of the finite thickness of the film, the transverse component of quasi-momentum is quantized. Therefore the electron/hole states assume quasidiscrete energy values in a thin film. As a consequence, the separation of valence and conduction bands increases by an amount E_z given by the above relation. The effective mass of holes calculated from the slope of the E_g vs. $1/t^2$ plot (assuming electrons to be heavy) is found to be 8.00×10^{-4} m_o where m_o is the electron rest mass. The de Broglie wavelength of the holes, estimated by taking the Fermi energy to be half of the average band gap, turns out to be about 1306 Å. Thus a quantum size effect is expected to be exhibited by the films, in the thickness range used, viz., 450 Å to 1900 Å, particularly in the lower part of the range.

Films ware also deposited at different substrate temperatures ranging from room temperature to 413 K. However, the band gap did not exhibit any systematic variation except for a general trend of increase.

4. Conclusion

The observed bandgap variation with the thickness of the films is the most significant of the results. The variation closely follows the quantum size effect in the low thickness range.

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