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Optical band gap of $Sn_{0·2}Bi_{1·8}Te_3$ thin films

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Abstract. **$Sn_{0·2}Bi_{1·8}Te_3$ 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 500–4000 cm^{-1}. From the optical absorption data the band gap was evaluated and studied as a function of film thickness and deposition temperature. The data indicate absorption through direct interband transition with a band gap of around 0·216 eV. The detailed results are reported here.**

Keywords. **Thin films; band gap; optical absorbance; film thickness; size effect.**

1. Introduction

The V_2–VI_3 (V_2 = Bi, Sb; VI_3 = 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 (Stolzerm *et al* 1986; Arivuoli *et al* 1988). Among these, Bi_2Te_3 is the most potential material for thermoelectric devices such as thermoelectric generators, thermocouples, thermo coolers and IR sensors with the best figure of merit near room temperature (Roy *et al* 1978; Jeon *et al* 1981; Rowe and Bandari 1981; Goodman 1985; Jansa *et al* 1992). It also finds application in electronic, microelectronic, optoelectronic and electromechanical devices (Sakia *et al* 1981; Stolzerm *et al* 1986). Its melting point is 573°C and is a *p*-type semiconductor. There have been various studies on the bulk and thin film characteristics of Bi_2Te_3 including optical and electrical properties (Guha Thakurta and Bose 1970; Testardi and Burstein 1972; Rahmankhan and Akhataruzzaman 1982; George and Pradeep 1985). The authors have reported electrical resistivity of thin films of $Sn_{0·2}Bi_{1·8}Te_3$ (Desai *et al* 2000). However, there is no report on the band gap study of $Sn_{0·2}Bi_{1·8}Te_3$ thin films. We hereby report the thickness dependence of optical band gap of $Sn_{0·2}Bi_{1·8}Te_3$ 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 623°C, i.e. 50°C above the melting point. After 48 h of mixing, the molten charge was slowly cooled to room temperature over a period of two days. Thin films of $Sn_{0·2}Bi_{1·8}Te_3$ 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 (1948) 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 500–4000 cm^{-1}. The absorption coefficient was calculated as a function of photon energy from absorbance vs wavelength curve. The plots of $(ahn)^2$ vs hn were used to evaluate the optical gaps. A typical plot is shown in figure 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 zero of the ordinate is also indicated in the figure. The band gaps, E_g, were evaluated in this way for films of different thickness, t. The band gap variation with film thickness follows the relation

$$E_z = \frac{\hbar^2 p^2}{2m^*}\frac{1}{t^2},$$

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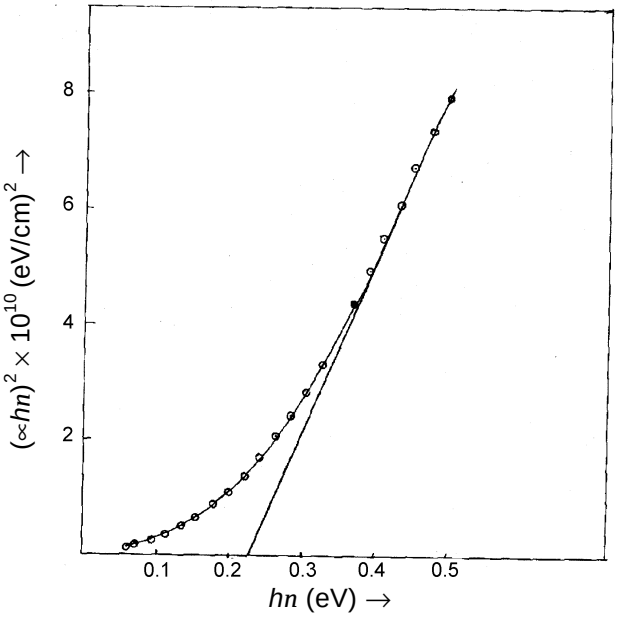

Figure 1. Plot of $(ahn)^2$ vs hn (film thickness = 1900 Å).

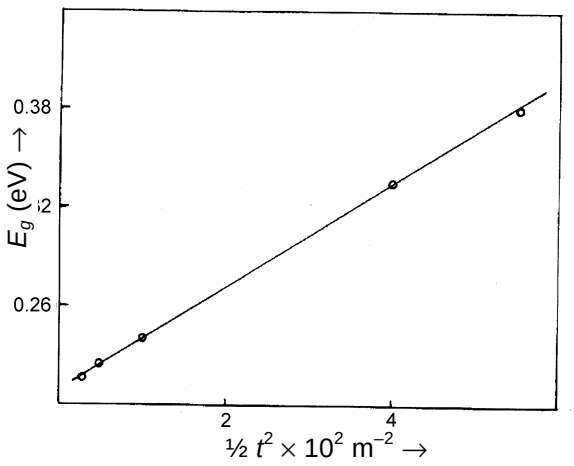

Figure 2. Plot of E_z vs $1/t^2$.

where m^* is the effective mass of the charge carrier, t the thickness of the film and E_z 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 (figure 2). This variation can be explained in terms of quantum size effect. This is usually defined as the 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 (Chopra 1969; Damodardas and Karunakaran 1983). 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 $0{\cdot}119 \times 10^{-4}\ m_0$, where m_0 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 1090 Å. Thus a quantum size effect is expected to be exhibited by the films, in the thickness range used viz. 450–1900 Å, particularly in the lower part of the range.

Films were 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. Conclusions

The following main conclusions can be drawn from the present study.

(I) Thin films of $Sn_{0{\cdot}2}Bi_{1{\cdot}8}Te_3$ are observed to have a direct band gap of about 0·216 eV.
(II) The films with thicknesses of about 1900 Å or less exhibit a quantum size effect with respect to optical absorption.
(III) The deposition temperature does not have a substantial effect on the optical band gap in these films.

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