RESEARCH PAPER | Physics | Volume : 6 | Issue : 3 | March 2016 | ISSN - 2249-555X | IF : 3.919 | IC Value : 74.50

Optical Properties of $Sn_{0.5}Se_{2.5}$ Single Crystals

KEYWORDS: $Sn_{0.5}Se_{2.5}$ single crystal, optical absorption, energy band gap

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ABSTRACT *The single crystals of $Sn_{0.5}Se_{2.5}$ were grown by chemical vapour transport technique using iodine as a transporting agent. The grown crystals were characterized with the help of energy dispersive analysis by X-ray (EDAX), which gives confirmation about its stoichiometry. The band gap of $Sn_{0.5}Se_{2.5}$ single crystals was determined by optical absorption method. The measurement of this crystal was taken at room temperature near the fundamental edge of absorption. This spectrum was obtained by UV-VIS-NIR spectrophotometer in the range of 700 nm–1400 nm. Results have been analyzed on the basis of two and three-dimensional model. Both direct and indirect transitions are involved in the absorption process. The indirect transition was found to be allowed with two phonons involved in the process. The direct as well as indirect energy gaps and phonon energies for this crystal has been estimated. The results obtained are discussed in detail.*

INTRODUCTION

The optical properties of layered compounds have been the subject to considerable interest [1-4] for over a decade, because of the characteristics of a two dimensional crystals structure which leads, in many cases, to highly anisotropic physical properties. However, despite the important application of these compounds, i.e. for uses such as cathodic materials in lithium batteries, their optical properties have not yet been investigated sufficiently thoroughly.

The optical and electrical properties of tin monoselenide SnSe and tin dichalcogenides SnX_2 has been studied by Julien [5]. The semiconducting character of the single crystals is investigated by means of resistivity and Hall Effect in the temperature range from 90 to 300K. The energy gap data are obtained by absorption measurements. Raman scattering and infrared absorption spectra of lithium intercalated SnS_2 single crystals were recorded as a function of temperature in the frequency range 50-600 cm^{-1}. The new bands are interpreted such as modes due to vibrations of lithium atoms located in the van der Walls gap against the nearest neighboring chalcogen atoms [6]. The structural properties of transition metal dichalcogenide single crystals were studied [7-10]

2. Experimental

The single crystals of tin diselenide ($Sn_{0.5}Se_{2.5}$) were grown by the chemcial vapour transport (CVT) technique. The stoichiometry of as grown crystals were confirmed with the help of Energy Dispersive Analysis by X-ray (EDAX). Thin samples for absorption measurement were obtained by cleavage. The 'a' and '*b*' axes were contained in the plane of cleavage. The optical absorption data were obtained by means of UV-VIS-NIR Spectrophotometer (Make: Perkin Elmer, Model: Lambda –19). All measurements were taken at room temperature with the electric field of the incident light parallel to the '*a*' and '*b*' crystallographic axes, respectively. Measurement along the c-axis were not performed because the crystal structure did not permit cutting and polishing. The energy range of incident photons was extended from 1.0 to 2.5.

For obtaining the absorption spectra using UV-VIS-NIR spectrophotometer from single crystal specimens, thin flakes of as grown crystals are used. These flakes are pasted on a thick black paper with a cut exposing the crystal flake to the incident light. The reference used is a replica of the black paper, having the cut at exactly the same position as the specimen. This arrangement is necessary because the crystal size is smaller than that of the sample compartment. Blank glass slides can also use as replica. For reflectance measurement standard aluminum coated mirror can be used as reference. The optical absorption spectrum of as grown crystals is shown in **Figure 1.**

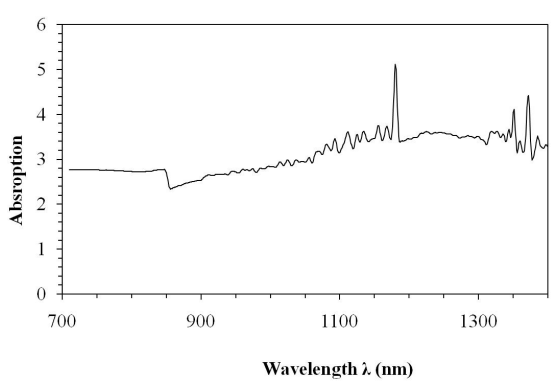

Figure 1: Absorption spectra of $Sn_{0.5}Se_{2.5}$ single crystals.

RESULT & DISCUSSION

The absorption spectrum was taken over the spectral range of 700 - 1400 nm. The interpretation of experimental results, viz the dependence of absorption coefficient 'α' in terms of the direct and indirect transitions is most often performed with the help of formula derived for three dimensional (3D) crystals. Their simplest form is as follow [11],

For direct band gap $$\alpha h\upsilon = A(h\upsilon - E_g)^r \quad (1)$$

For indirect band gap $$\alpha h\upsilon = \sum_j B_j (h\upsilon - E_g' \pm E_p)^r \quad (2)$$

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Here 'α' is absorption coefficient, calculated as a function of photon energy from absorption vs wavelength curve. hν is the energy of the incident photon, E_g the energy for the direct transition, E'_g the energy for the indirect transition and E_{pj} the energy of the phonons assisting at indirect transition. A and B are parameters depending in the more complicated way on temperature, photon energy and phonon energies E_p.

Figure 2 shows the spectral variation of $(ahν)^{1/2}$ vs hν. Since the curve indicates a discontinuous straight line it is quite possible that it represents indirect interband transition involving the emission or absorption of phonon. In order to make an accurate determination of the points of discontinuities, the method used which was adopted by earlier researchers [12]. The band gap was obtained by extrapolating the linear part to the energy axis for zero absorption. The graph of $\delta (ahν)^{1/2}$ / dhν versus hν has been shown in **Figure 3**. It can be clearly seen that the derivation are step function of energy with four steps well defined in the range $E_1 < E < E_2$, $E_2 < E < E_3$, $E_3 < E < E_4$ and $E_4 < E$. The values of E_1, E_2, E_3 and E_4 indicate the points of discontinuities and shown in the plot of $\delta (ahν)^{1/2}$ / dhν versus hν. The indirect energy gap obtained from these values of E_1, E_2, E_3 and E_4 are given by

$$E'_g = \frac{E_1 + E_4}{2} = \frac{E_3 + E_2}{2} \quad (3)$$

and the phonon energies are given by

$$Ep_1 = \frac{E_4 - E_1}{2} \text{ And } Ep_2 = \frac{E_3 - E_2}{2} \quad (4)$$

The phonon equivalent temperature (θ_i) is a defined by the equation,

$$\theta_i = \frac{E_{pi}}{k} \quad (5)$$

where E_{pi} being the i^{th} phonon energy.

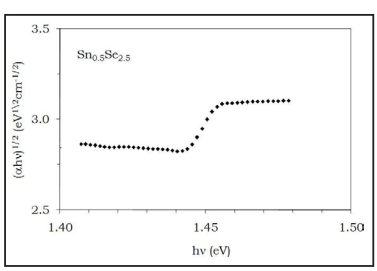

Figure 2: The plot of $(ahν)^{1/2}$ vs photon energy (hν) for $Sn_{0.5}Se_{2.5}$ single crystal.

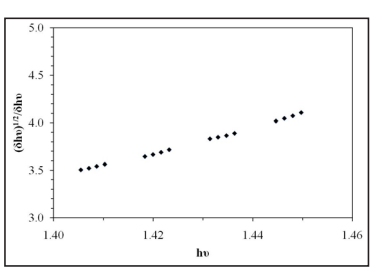

Figure 3: The graph of $\delta(ahν)^{1/2}/dhν$ *vs. hn*

The obtained values of indirect band gap, phonon energies and phonon equivalent temperature are shown in **Table 1**. For the determination of direct gap, the best fit of all the experimental points was observed in the case of a $(ahν)^2$ vs hν plote which is shown in **Figure 4**. The values of E_g obtained from the intercept of the straight line portion of the curve on the 'hν' axis are as shown in Table 1.

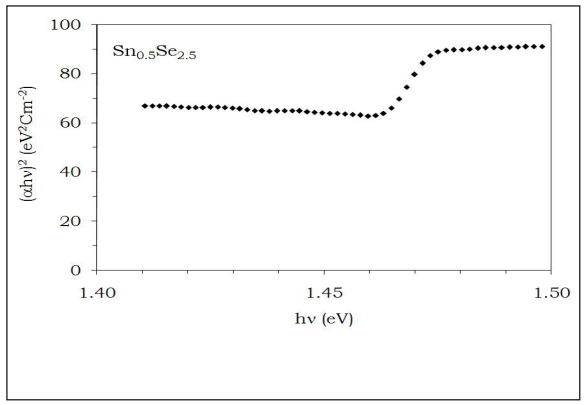

Figure 4: The plot of $(ahν)^2$ vs photon energy (hν) for $Sn_{0.5}Se_{2.5}$ single crystal.

Table 1: The values of band gap and phonon energies of $Sn_{0.5}Se_{2.5}$ single crystals

Parameter	Obtained values
E_1 (eV)	1.4103
E_2 (eV)	1.4232
E_3 (eV)	1.4363
E_4 (eV)	1.4497
E'_g (C) (eV)	1.4300
E'_g (E) (eV)	1.4300
E_{p1} (meV)	19.7
E_{p2} (meV)	6.55
q_1 (K)	228.69
q_2 (K)	76.037
E_g (e V) (Direct)	1.442

CONCLUSION

In this paper authors observed that both direct as well as indirect symmetry allowed transitions gives a good account of the optical absorption edge in as grown single crystals. In this context, authors have come to the following conclusions:

The chemical vapour transport (CVT) technique is most suitable for the growth of large size single crystals of $Sn_{0.5}Se_{2.5}$.

The energies of the direct band gap for this crystal have been determined.

The accurate analysis of the data shows that the indirect transition represented by the absorption curves is indirect allowed involving two different phonons. The energies of these phonons have been determined.

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