

Optical band gap studies on Zn-Te pellets

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Spectroscopic techniques are very useful for characterizing semiconducting and conducting materials. The optical properties (specially reflection spectra) of $\text{Zn}_x\text{Te}_{100-x}$ ($x=5, 10, 30$ and 50) material in pellet form were studied. Polycrystalline semiconducting material has been prepared by Melt quenching method by taking pure Zn and pure Se in appropriate atomic weight ratio. The polycrystalline nature of $\text{Zn}_5\text{Te}_{95}$ was confirmed by XRD studies. In order to compare the studies on so prepared polycrystalline material and commercially obtained pure $\text{Zn}_{50}\text{Te}_{50}$ material, investigations were carried out on both types of samples. From the analysis of reflection spectra, energy band gaps of $\text{Zn}_x\text{Te}_{100-x}$ material have been determined, which were found to increase from 1.67 to 2.31 eV. It is observed that the optical band gap of laboratory prepared $\text{Zn}_{50}\text{Te}_{50}$ material is in excellent agreement with that of commercially obtained pure $\text{Zn}_{50}\text{Te}_{50}$ material.

Keywords: Polycrystalline semiconducting material, Reflection spectra, Spectrophotometer, Energy band gap

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1 Introduction

Great attention has been given to II-VI group chalcogenide materials, in recent years, mainly due to their wide range applications as solid-state devices both in scientific and technological field. These materials have come under increased scrutiny because of their wide use in cost reduction of devices for photovoltaic applications¹. The research on renewable energies includes the photovoltaic conversion of solar energy and important investigations of novel materials and structures². Photovoltaic methods are one of the most fascinating ways for direct solar energy conversion³. ZnTe is the most suitable semiconducting material to achieve this goal. It has been investigated for its uses as visible light-emitting semiconductor laser⁴.

ZnTe is a potentially low cost semiconductor for switching devices and multi-junction solar cells. ZnTe, being a wide and direct band gap (2.26 eV) semiconducting material with low electronic affinity (3.53 eV), can absorb photons in the visible region without any phonon assisted mechanism and that makes it useful in several electro-optic and opto-electronic applications. Recent advancements in solar cell technology have indicated that ZnTe and its alloys may effectively be used in CdTe based solar cells. Polycrystalline ZnTe material and its alloys like

CdZnTe were successfully utilized in the fabrication of tandem solar cell structures with a tailored band gap and quantum well structures. All these created a renewed interest in the studies of ZnTe material for the fabrication of devices⁵.

Most of the devices have been fabricated by making use of thin film of these materials, which however proved to be low lifetime devices with respect to their thermal degradation, and no serious efforts have been made to prepare the material in bulk form to produce such devices. Though, absorption spectra technique is used in case of thin films⁶, reflection spectra technique is used for bulk material in the present work. In view of this, an investigation has been undertaken to study the optical band gap of $\text{Zn}_x\text{Te}_{100-x}$ ($x=05, 10, 30$ and 50) system in pellet form using Hitachi spectrophotometer in the wavelength range from 450 to 800 nm. Optical band gap of a pellet of commercially obtained pure $\text{Zn}_{50}\text{Te}_{50}$ material has also been determined by the same technique in order to compare the result of our laboratory prepared sample. X-ray diffraction (XRD) has also been performed in $\text{Zn}_5\text{Te}_{95}$ for its structural analysis.

The main aim to carry out above study is to know that how structural and optical properties change in the Te, when it is mixed with Zn at different

concentrations. Where the knowledge of the optical properties of chalcogenide semiconductors is, indeed, necessary for exploiting all their technological potential⁷.

2 Experimental Details

2.1 Sample preparation

Zn_xTe_{100-x} alloys were prepared by using melt-quenching method. High purity (99.99%) tellurium granules and fine Zn dust in appropriate atomic percentage were weighed in a quartz glass ampoule (length 5 cm and internal diameter 8 mm). The content of the ampoule was sealed in a vacuum of 10⁻⁶ Torr and heated in a furnace where temperature was raised at a rate of 3-4 K per minute up to (1070 ± 2) °K and kept around at that temperature for 10 h. The ampoules were hand shaken to obtain the homogeneity of the samples. The molten samples were then rapidly quenched in ice cooled water. Then pellets of thickness 2 mm and diameter 12 mm were prepared from the powder of the samples at a constant load of 5 tons (4.33 × 10⁸ Pa) in a hydraulic press.

2.2 Structural and optical characterization

X-ray diffractometer (Philips PW 1830) was employed to obtain X-ray diffractogram of Zn₅Te₉₅ material at room temperature. This diffractogram was analyzed to obtain crystallographic information on these samples. The copper target was used as a source of radiation. The scanning angle (2θ) was in the range of 20-80°.

The optical reflectance⁸ of pure ZnTe pellet and Zn_xTe_{100-x} (x= 5, 10, 30 and 50) were recorded at room temperature in the wavelength range from 450 to 800 nm using a Hitachi (Japan) double-beam-spectrophotometer. In this model, the prism/grating double monochromatic system is used. The optical band gap of the pellet was determined with the help of reflection spectra. Since it has not been possible to get transmission spectra of ZnTe pellets due to high absorption, the reflection spectra for determination of optical band gap have been recorded. To include the effect of reflection from upper surface of the pellet a mirror is placed on top of the pellet and reflection spectra are recorded. According to Tauc relation⁹, the absorption coefficient for direct band gap material is given by

$$\alpha \text{ } hv = A(hv - E_g)^{1/2} \quad \dots (1)$$

where $h\nu$ is photon energy, E_g the band gap and A is constant which is different for different transitions.

The absorption coefficient α may be written in terms of reflectance¹⁰ as,

$$2 \alpha t = \ln[(R_{\max} - R_{\min}) / (R - R_{\min})] \quad \dots (2)$$

where t is thickness of pellet and R is reflectance for any intermediate photon energy. A sudden fall in reflectance from R_{\max} to R_{\min} is observed due to the absorption of light by the material. A graph between $[h\nu \ln\{(R_{\max} - R_{\min}) / (R - R_{\min})\}]^2$ (as ordinate) and $h\nu$ (as abscissa) is plotted and, a straight line is obtained. The extrapolation of straight line to $h\nu$ axis gives the value of band gap of the material of the pellet.

3 Results and Discussion

3.1 Structural properties

The X-ray diffraction pattern gives valuable information about the nature and structure of the material. The presence of sharp structural peaks in XRD patterns confirmed the polycrystalline nature of the material. The experimental d -values for Zn₅Te₉₅ material have been calculated from Bragg's relation, $2d\sin\theta = n\lambda$, by taking the θ values from the peaks of XRD pattern¹¹. These calculated d -values are compared with d^* -values obtained from ASTM data for ZnTe and Te. The experimental d -values of ZnTe and Te in Zn₅Te₉₅ materials are in good agreement with the ASTM d^* -values of ZnTe and Te.

Figure 1 shows the XRD trace of the sample material containing ZnTe and Te and Table 1 gives the comparison of XRD data with ASTM data for different (h k l) values. On the basis of these results the identification of different peaks appearing in the XRD trace has been carried out. The peaks are due to ZnTe and unreacted Te, where the ZnTe is present in cubic structure and Te has hexagonal structure, as indicated by the ASTM data for Te and ZnTe. The Te fraction is dominant in this sample. The presence of sharp structural peaks in XRD pattern confirms the polycrystalline nature of the material. These studies also suggest about the presence of large amount of Te at lower percentage of Zn.

3.2 Optical properties

Figure 2 represents the reflection spectra of freshly prepared Zn_xTe_{100-x} material and commercially obtained pure Zn₅₀Te₅₀ material in pellet form. We have plotted the graph between % R and wavelength, λ (nm), it is observed from Fig. 2 that reflection decreases with the decrease in λ . A sharp fall present at a particular wavelength, indicates the presence of optical band gap in these samples.

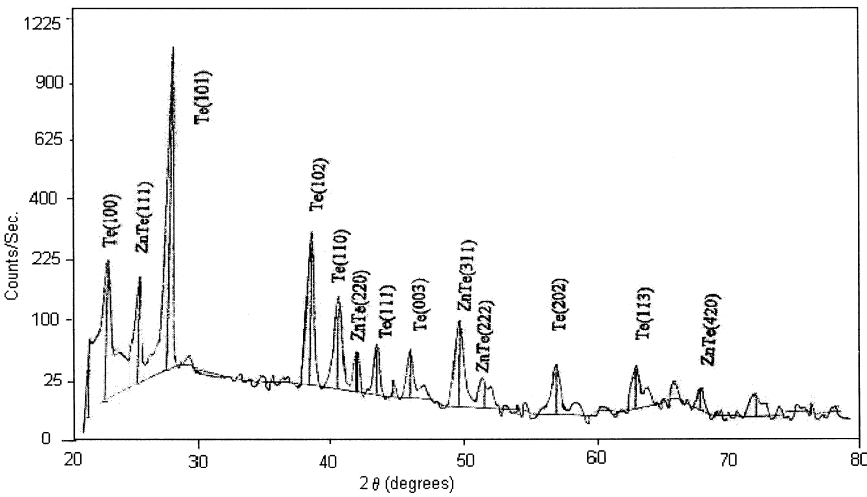


Fig. 1—X-ray diffraction pattern of Zn₅Te₉₅ material.

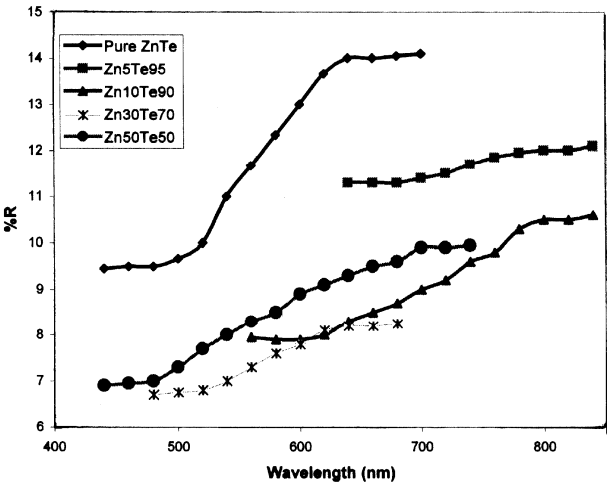


Fig. 2—Reflection spectra of Zn_xTe_{100-x} material and pure Zn₅₀Te₅₀ material.

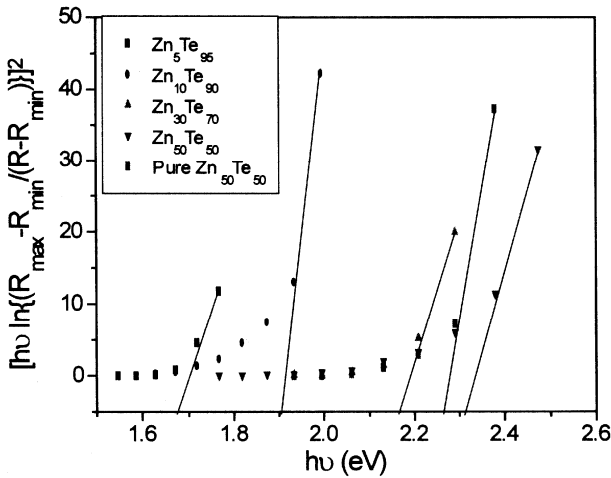


Fig. 3—Band gap determination of Zn_xTe_{100-x} material and pure Zn₅₀Te₅₀ material.

Table 1—Analysis of X-ray diffraction data of Zn₅Te₉₅

2θ	Relative Intensity%	d(Å) Exp.	d*(Å) ASTM	hkl	Identification
22.99	20.81	3.8638	3.86	100	Te
25.27	15.80	3.5214	3.523	111	ZnTe
27.57	100	3.2328	3.230	101	Te
38.28	27.72	2.3493	2.351	102	Te
40.43	12.59	2.2291	2.228	110	Te
41.86	3.94	2.1562	2.159	220	ZnTe
43.34	5.14	2.0806	2.087	111	Te
45.92	4.67	1.9745	1.980	003	Te
49.60	9.62	1.8364	1.840	311	ZnTe
51.51	1.89	1.7727	1.762	222	ZnTe
56.91	3.95	1.6168	1.616	202	Te
62.90	3.21	1.4763	1.479	113	Te
67.79	1.46	1.3813	1.3645	420	ZnTe

Tauc relation as given in Eq. (2) is used for the determination of energy band gap shown in Fig. 3. Graphs have been plotted between the square of $hv \ln[(R_{\max} - R_{\min}) / (R - R_{\min})]$ and hv for determination of energy band gap. On comparing the band gap values of commercially obtained and laboratory prepared Zn₅₀Te₅₀ materials, it is observed that both are in good agreement. Which indicates that the reflection spectra technique used is useful to determine the band gap of bulk materials.

A graph between Zn concentration and optical band gap has been plotted in Fig. 4. The optical band gap shows an increasing nature. At lower Zn concentration this increase is very sharp. Towards the higher Zn concentration, band gap starts assuming a

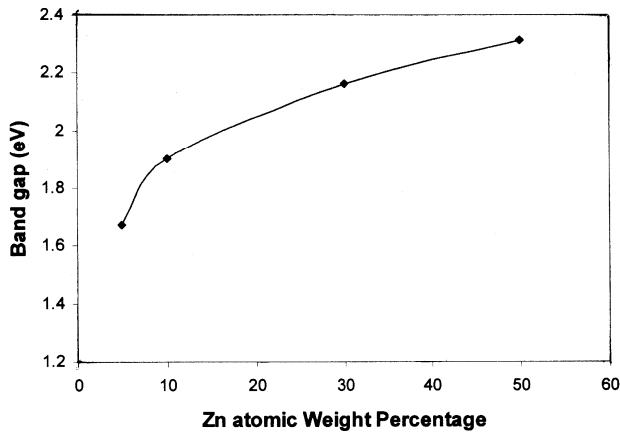


Fig. 4—Band gap versus Zn atomic weight percentage.

constant value. When Zn is added to Te, the formation of ZnTe takes place and band gap increases, since the band gap of ZnTe is larger than Te. The band gap of amorphous Te films¹² and the ZnTe semiconducting material⁵ is 0.8 eV and 2.26 eV, respectively. So, formation of ZnTe is the basis of increase of band gap. This might be due to the fact that, addition of Zn into Te, produces a change in lattice of Te in the sample. XRD data suggests that, Te has hexagonal lattice structure, whereas the lattice structure of ZnTe is cubic. So, with the increasing Zn concentration in Te, the formation of ZnTe takes place and hexagonal structure of Te transforms to cubic structure of ZnTe, as indicated by the ASTM data of Te and ZnTe. Thus, with the increase of contents of ZnTe in the system, the energy band gap also increases.

4 Conclusions

(1) In highly absorbing samples where transmission spectroscopy cannot be used for determination of energy band gap of samples like in pellets, reflection spectroscopic technique with slight modification has proved to be useful method.

(2) XRD trace of the sample prepared by melt quenching method shows polycrystalline nature of the sample. It has been noticed that for the given

concentrations of Zn samples of Zn-Te do not form a glass. This is suggestive of the fact that when the melt of the $\text{Zn}_x\text{-Te}_{100-x}$ in the ampoule is cooled down the motion of the atoms is not arrested and crystallization stands at the same time.

(3) The energy band gap increases with the increase of Zn concentration. At lower Zn concentration this increase is sharp and tends to saturate towards higher Zn concentration.

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