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INFLUENCE OF COMPOSITION ON THE OPTICAL BAND GAP IN *A*-$Ge_{20}Se_{80-X}In_X$ THIN FILMS

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Thin films of $Ge_{10}Se_{80-x}In_x$ ($x = 0, 5, 10, 15, 20$) bulk material were prepared by thermal evaporation technique at a base pressure of $\sim10^{-6}$ mbar. Amorphous nature of the bulk and deposited thin films was confirmed by x-ray diffraction technique. Optical transmission spectra of the films were taken in the range of 400-1200 nm. The optical band gap was determined and the variation in the band gap is explained in terms of average bond energy of the system.

Keywords: Chalcogenide glasses, absorption coefficient, optical band gap, average bond energy

1. Introduction

The physical properties of chalcogenide glasses have attracted much interest due to their wide technical applications [1]. Besides, the physical properties of chalcogenide semiconducting glasses are strongly dependent on their compositions [2,3]. Chalcogenide semiconductors have truly emerged as multipurpose materials and have been used to fabricate technological important devices such as infrared detector, electronic and optical switches and optical recording media [4]. Such wide-ranging applications are possible due to some unique phenomena like photoinduced structural transformations [1]. In recent years, efforts are being made to develop chalcogenide based erasable optical storage media. Thermal processes are known to be important in chalcogenide glasses. Recently, thin films of amorphous chalcogenide glasses [5] have been studies as materials for phase change optical storage.

It has been reported that amorphous Se has special interest because of its device applications such as rectifiers, photocells, xerography, switching and memory devices etc. [9]. In the pure state, it has disadvantages because of its short lifetime and low sensitivity. To overcome this difficulty, several workers [6–9] have used certain additives (Ge, Te, Bi, Sb, As, etc.) to make binary alloys with selenium, which in turn gives high sensitivity, a high crystallization temperature and smaller aging effects. The addition of third element (In) expands the glass forming area and also creates compositional and configurational disorder in the system [10–12].

The present work deals with the study of absorption coefficient and optical band gap in $Ge_{10}Se_{80-x}In_x$ ($x = 0, 5, 10, 15, 20$) thin films. The transmission spectrum of the thin films is taken in the range of 400-1200 nm.

2. Experimental procedure

Bulk samples $Ge_{20}Se_{80-x}In_x$ ($x = 0, 10, 15, 20$) were prepared by melt quenching technique. The materials (5N pure) were weighed in accordance with their atomic weight percentage. The weighed materials were sealed in evacuated ($\sim10^{-6}$ mbar) quartz ampoules and heated up to 1000

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^{0}C in a rocking furnace at a heating rate of 3-4 ^{0}C/min. Ampoules were frequently rocked at the highest temperature for 10 hours. The quenching was done in ice cold water immediately after taking out the ampoules from the furnace. The amorphous nature of the bulk samples was confirmed by the x-ray diffraction technique as no sharp peak was observed. Thin films of the bulk samples were prepared on cleaned glass substrates by thermal evaporation technique [Vacuum coating unit HINDHIVAC 12A4D Model] at base pressure of ~ 10^{-6} mbar. Amorphous nature of thin films was also checked by x-ray diffraction technique. The normal incidence transmission spectra of $Ge_{20}Se_{80-x}In_x$ ($x = 0, 5, 10, 15, 20$) thin films have been taken by a double beam UV-VIS-NIR spectrophotometer [Hitachi-330] in the transmission range 400-1200 nm. The spectrophotometer was set with a suitable slit width of 1 nm in the measured spectral range. All measurements were taken at room temperature (300K).

3. Results and discussion

The optical system under consideration is amorphous, homogeneous and uniform. Optical transmission is a very complex function and is strongly dependent on the absorption coefficient (α). Fig. 1 shows the transmission spectrum of a-$Ge_{20}Se_{80-x}In_x$ ($x = 0, 10, 15, 20$) thin films. The oscillating nature of the spectrum shows that the films are having uniform thickness.

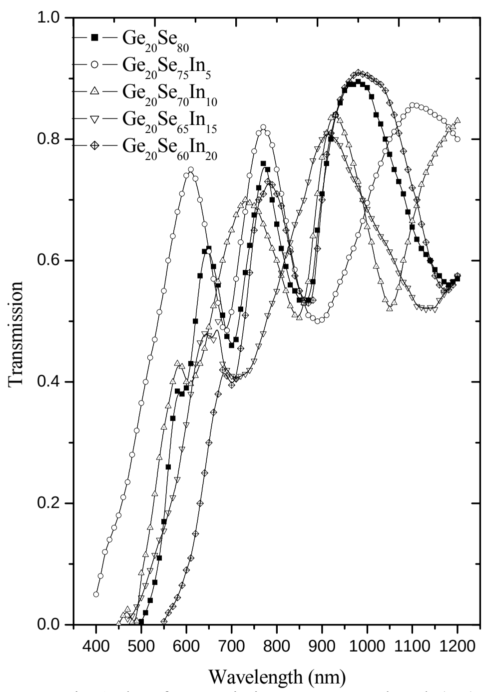

Fig. 1 Plot of Transmission versus Wavelength (nm) for $Ge_{20}Se_{80-x}In_x$ thin films

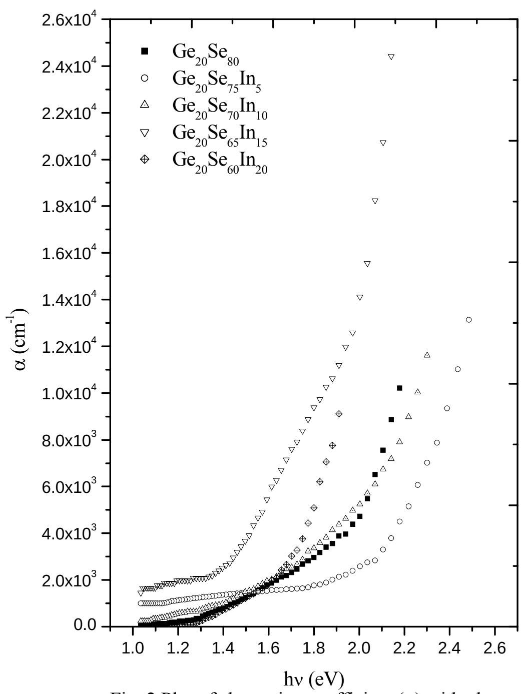

Fig. 2 Plot of absorption coefficient (α) with photon energy (hν) for $Ge_{20}Se_{80-x}In_x$ thin films

The absorption coefficient of the thin films is calculated by using the expression

$$\alpha = (1/d)\ln(1/x)$$

where d is the thickness of the thin film and x is the absorbance [13]. The variation of absorption coefficient with the photon energy is shown in Fig. 2.

The optical band gap has been estimated from absorption coefficient data as a function of wavelength by using Tauc Relation [14]

$$\alpha h\nu = B\left(h\nu - E_g^{opt}\right)^n$$

where $h\nu$ is the photon energy, α is the absorption coefficient, E_g^{opt} the optical band gap, B is band tailing parameter and $n = 1/2$ for direct band gap and $n = 2$ for indirect band gap. This is observed from the plot (not shown here) between $log\ (\alpha h\nu)$ and $log\ (h\nu)$ that the nature of graph is non linear which shows that transition in the forbidden gap is indirect in nature [15].

Fig. 3 shows the variation of $(\alpha h\nu)^{1/2}$ with $h\nu$. Optical band gap E_g^{opt} can be determined by the extrapolation of best fit line between $(\alpha h\nu)^{1/2}$ and $h\nu$ to intercept the $h\nu$ axis ($\alpha = 0$) for $x = 0, 5, 10, 15, 20$ in $Ge_{20}Se_{80-x}In_x$ system.

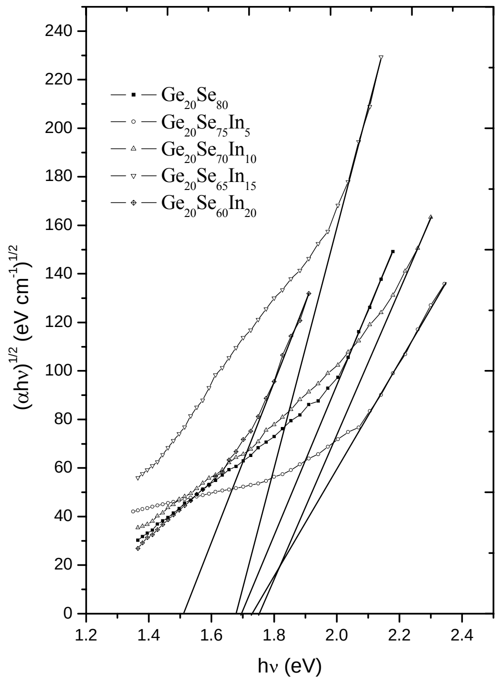

Fig. 3 Plot of $(\alpha h\nu)^{1/2}$ versus $h\nu$ for $Ge_{20}Se_{80-x}In_x$ thin films

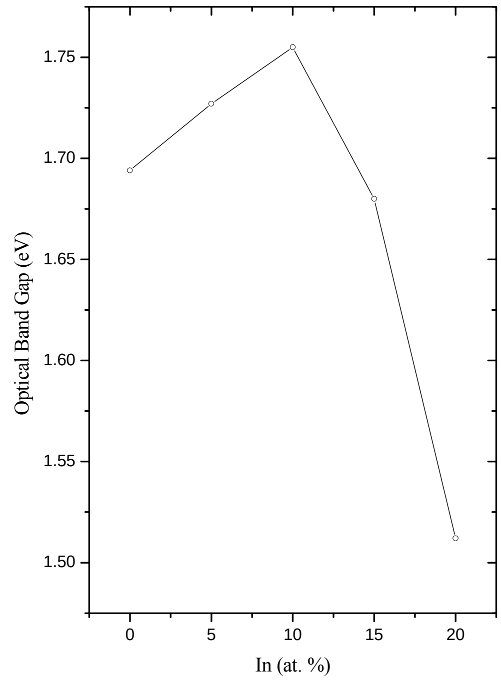

Fig. 4 Plot of optical band gap versus In content

Fig.4 shows graphically the variation of optical band gap with increasing %age of indium content. It is found that the optical band gap increases with increase in concentration of indium up to 10 at. % and at higher concentration of Indium (>10 at.%), it decreases. The Indium additives in $Ge_{20}Se_{80-x}In_x$ must bring about a compositional change of host network of Ge-Se i.e. the alloying effect, as the optical band gap is found to vary with indium concentration. This change in optical band gap may be understood in terms of the structure of Ge-Se system or on the basis of the change in average bond energy as a function of composition. According to Philips [16], molecular structure of melt-quenched Ge_xSe_{100-x} is much more ordered and may be expected from a continuous random network model. According to Phillips, Ge_xSe_{100-x} alloys may be described by chemically ordered clusters embedded in a continuous network. Some of these clusters are $(Se)_n$ chains, $Ge(Se_{1/2})_4$ corner sharing tetrahedral and $Ge_2(Se_{1/2})_6$ ethane like structural units. First two types dominate for $x \leq 33$ and third type is expected to occur at higher concentration of Ge i.e. $x > 33$. In our present system $a\text{-}Ge_{20}Se_{80-x}In_x$, Ge is 20 at. %, hence first two are possible. At lower concentration of Indium (up to 10 at.%), Indium atoms may enter into Se chain resulting in the systematically replacement of Se-Se bond having bond energy of 206 $KJmol^{-1}$ with Se-In bonds having a bond energy of 257.5 $KJmol^{-1}$. Since energy of Se-In bond is higher than Se-Se bond, the average bond energy of the system increases. Since optical band gap is a bond sensitive property [17], an increase in the average bond energy results in the increase in optical band gap in $Ge_{20}Se_{80-x}In_x$ at $x = 0, 10$ at. % thin films. At higher concentration of Indium at $x = 15, 20$ at. %, Indium enters into Ge-Se system. Since Ge remains constant, so replacing Se with Indium results in the reduction of Ge-Se bonds having single bond energy of 205.2 $KJmol^{-1}$ and increase of Ge-In bonds is having single bond energy of 146.06 KJmol^{-1}. This reduction in average bond energy of system $Ge_{20}Se_{80-x}In_x$ at $x = 15, 20$ is reflected in reduction of the optical band gap.

4. Conclusion

Optical band gap of the thin films of $Ge_{20}Se_{80-x}In_x$ ($x = 0, 5, 10, 15, 20$) has been calculated using the transmission spectrum in the range 400-1200 nm. The optical band gap was found to increase first up to 10 at. % addition of Indium and thereafter it decreases. This behavior is explained on the basis of average bond energy of the system.

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