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Effect of Cu incorporation on the optical parameters of $Se_{75}Te_{25}$ thin film

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Amorphous thin films of $Se_{75}Te_{25-x}Cu_x$ (x = 0 & 10) have been deposited onto chemically cleaned glass substrate by thermal evaporation technique in the presence of vacuum. The optical parameters like refractive index (n), extinction coefficient (k), absorption coefficient (α), real and imaginary dielectric constants (ε' & ε") have been calculated in the wavelength range 400-2100 nm by Swanepoel method using optical transmission data. It is observed that extinction coefficient (k) and imaginary dielectric constants (ε") decrease with increase in wavelength (λ). The absorption coefficient (α) increases with photon energy (hν). It is also found that refractive index (n) decreases and extinction coefficient (k), absorption coefficient (α), imaginary dielectric constants (ε") increases with Cu content. The optical band gap (E_g) has also been calculated by Tauc's relation and found to decrease with Cu content in $Se_{75}Te_{25-x}Cu_x$ system. The results are interpreted in terms of change in the density of localized states (DOS).

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1. Introduction

Chalcogenide glasses have attracted lot of attention in the field of electronics as well as in optics due their peculiar properties suitable for processing of devices for electrical switching and memories, optical memory applications, x-ray imaging etc. These materials in particular selenium exhibit a unique property of reversible transformation [1], which makes these glasses useful as optical memory devices. The effect of alloying Te into a-Se [2-5] has been reported and it is found that the incorporation of Te results in dissociation of long polymeric chains and eight member rings of amorphous selenium [6]. This makes Se-Te alloys more important as compared to a-Se due to distinct advantages (greater hardness, better photosensitivity, lesser ageing effects etc.) and hence find applications as recording layer material in optical phase change technique [7]. However, in these alloys limited reversibility [8] and low glass transition and crystallization temperatures are serious drawbacks.

These drawbacks can be overcome by addition of third element as a chemical modifier as it is reported to expand the glass forming region and also creates compositional and configurational disorder [9-13], which play a major role in device preparation. Thus incorporation of third element Cu to Se-Te binary alloy is expected to modify the structure of the host alloy. Therefore the optical transmittance of thin films of $Se_{75}Te_{25-x}Cu_x$ alloy is interesting to study in detail from basic as well as application point of view.

In the present work, the optical transmission spectra of thin films of $Se_{75}Te_{25-x}Cu_x$ (x = 0 & 10) are measured in the wavelength range 400-2100 nm by spectrophotometer (Perkin-Elmer, model Lambda-750). If the thickness d is uniform, interference effects give rise to the spectrum showed a maxima and minima of the transmission curve. These interference fringes can be used to calculate various optical parameters. Therefore, we have calculated optical band gap and other optical parameters like refractive index (n), extinction coefficient (k), absorption coefficient (α), real and imaginary dielectric constants (ε` & ε") for $Se_{75}Te_{25-x}Cu_x$ system.

Section 2 and 3 describes the experimental details and the results respectively. The conclusions have been presented in the last section.

2. Experimental details

2.1 Sample preparation

Bulk samples of $Se_{75}Te_{25-x}Cu_x$ (x = 0 & 10) system were prepared by melt quenched technique. High purity elements (99.999 %pure), selenium, tellurium and copper were weighed by electronic balance (Shimadzu, AUX 220) according to their atomic percentages, with a least count of 10^{-4} gm. The properly weighed materials were put into clean quartz ampoules (length ~ 5 cm and internal diameter ~ 8 mm) and then sealed under vacuum of 1.3×10^{-3} Pa. These sealed ampoules were heated in electric furnace up to 1000°C and kept at that temperature for 10 - 12 hours. The temperature of the furnace was raised slowly at a rate of 3-4 °C/min. During the heating process ampoules were constantly rocked, by rotating a ceramic rod to which the ampoules were tucked away in the furnace. This was done to obtain homogenous glassy alloy.

After rocking for about 10 hours, the obtained molten materials ampoules rapidly quenched by removing the ampoules from the furnace and dropping into ice-cooled water. The quenched samples of the glassy alloys were taken out by breaking the quartz ampoules. The glassy nature of samples was ascertained by the X-ray diffraction pattern. Compositional analysis was performed using electron probe micro- analysis (EPMA) technique.

Thin films of glassy alloys of $Se_{75}Te_{25-x}Cu_x$ were prepared by vacuum evaporation technique keeping glass substrate at room temperature. The thin films were kept in the deposition chamber in the dark for 24 hours before using them. This was done to allow sufficient annealing at room temperature so that a metastable thermodynamic equilibrium may be attained in the samples as suggested by Abkowitz [14].

2.2 Procedure of measurements

The normal incidence transmission spectra of $Se_{75}Te_{25-x}Cu_x$ thin films have been taken by a double beam UV-VIS-NIR spectrophotometer in the transmission range 400-2100 nm. The spectrophotometer was set with a suitable slit width of 1nm in the measured spectral range.

3. Results and discussion

Optical transmission is a very complex function and is strongly dependent on the absorption coefficient (α). Fig.1 shows the transmission spectrum as a function of wavelength for thin films of $Se_{75}Te_{25-x}Cu_x$ (x = 0 & 10) system.

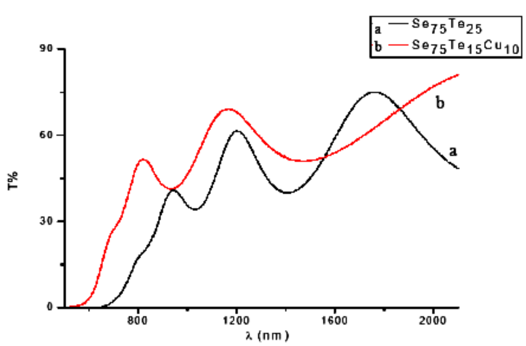

Fig. 1. Spectral distribution of the transmission (T%) with wavelength (λ) for $Se_{75}Te_{25-x}Cu_x$ thin films.

3.1. Determination of Optical parameters (a method of calculation)

The optical parameters (refractive index n, extinction coefficient k, absorption coefficient α) were determined using Swanepoel's method [15-18]. According to this method the transmission spectrum can roughly be divided into four regions. Interference fringes can be used to calculate the optical constants of the film. The basic equations for the various regions are as follow:

(i) For the transparent region the refractive index *n* is given by

$$n = [N+ (N^2-s^2)^{1/2}]^{1/2} \quad (1)$$

Where

$$N= (2s/T_m)-(s^2+1)/2 \quad (2)$$

T_m is the envelope function of the transmittance minima and s is the refractive index of the substrate.

(ii) The region of weak and medium absorption, the refractive index *n* is given by

$$n = [N + (N^2 - s^2)^{1/2}]^{1/2} \quad (3)$$

Where

$$N = [2 s (T_M-T_m) / T_M T_m] + (s^2+1) /2 \quad (4)$$

T_M is the envelope function of the transmittance maxima. For the extinction coefficient *k,* the absorbance, *x,* is given in terms of the interference extremes using the following relation:

$$x = [E_m-\{E_m{}^2-(n^2-1)^3(n^2-s^4)\}^{1/2}]/ [(n-1)^3(n-s^2)] \quad (5)$$

Where

$$E_m= [(8n^2s/ T_m) - (n^2-1) (n^2-s^2)] \quad (6)$$

And

$$x=\exp(-4\pi kd/\lambda) \quad (7)$$

(iii) For the region of strong absorption where the interference maxima and minima converge to a single curve, the absorbance, *x* is given by [18]:

(iv)

$$x= T_0 (n+1)^3 (n+s^2)/ 16n^2s \quad (8)$$

The spectral distribution of both n and k constants for $Se_{75}Te_{25}$ and $Se_{75}Te_{15}Cu_{10}$ films are shown in Fig. 2 and 3, respectively, and the calculated values are also given in Table 1.

Table 1. Optical parameters of $Se_{75}Te_{25-x}Cu_x$ thin film.

Samples	Refractive index (n)	Extinction coefficient (k)	Real dielectric constant (ε`)	Imaginary dielectric constant (ε'')	Film thickness(d) (nm)
$Se_{75}Te_{25}$	3.01	9.54×10^{-3}	9.09	5.69×10^{-2}	3200

$Se_{75}Te_{15}Cu_{10}$	2.66	1.19 x10^{-2}	7.06	6.31 x10^{-2}	2000

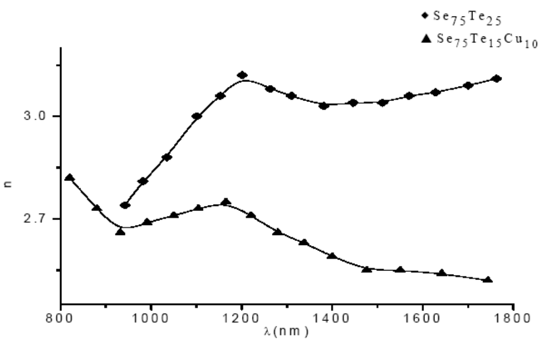

Fig. 2. Variation of refractive index (n) vs wavelength for $Se_{75}Te_{25-x}Cu_x$ thin films.

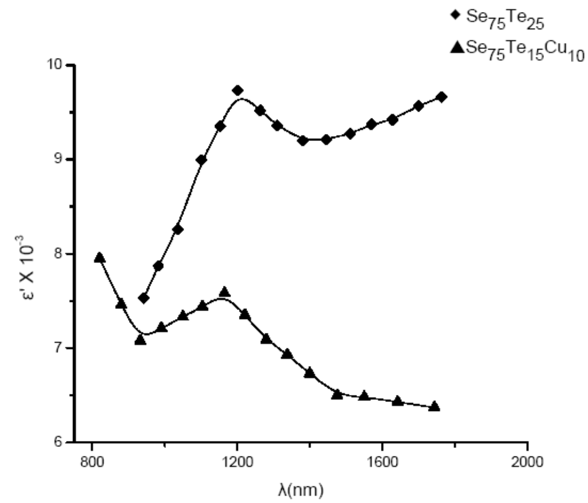

Fig. 4. Variation of real dielectric constant (ε') vs wavelength (λ) for $Se_{75}Te_{25-x}Cu_x$.

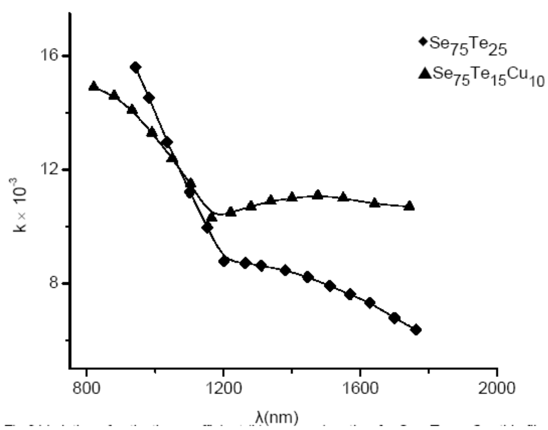

Fig. 3. Variation of extinction coefficient (k) vs wavelength (λ) for $Se_{75}Te_{25-x}Cu_x$ thin films.

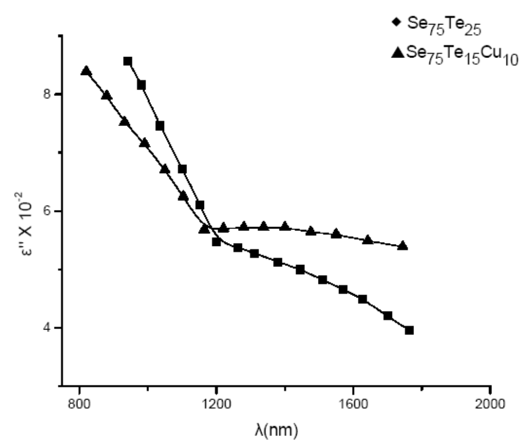

Fig. 5. Variation of imaginary dielectric constant (ε'') vs wavelength (λ) for $Se_{75}Te_{25-x}Cu_x$

3.2 Determination of dielectric constants

The dielectric constant of the films can be calculated with the help of refractive index n and extinction coefficient k [19]. Real dielectric constant (ε`) can be calculated by the relation,

$$\varepsilon` = n^2 - k^2 \tag{9}$$

While the imaginary dielectric constant (ε") can be calculated by the relation,

$$\varepsilon'' = 2nk \tag{10}$$

The spectral distribution of both real and imaginary dielectric constants for $Se_{75}Te_{25}$ and $Se_{75}Te_{15}Cu_{10}$ films are shown in Fig. 4 and 5, respectively, and the calculated values are also given in Table 1. It is found that refractive index (n) decreases and extinction coefficient (k), absorption coefficient (α), imaginary dielectric constants (ε") increases with Cu content.

3.3 Determination of absorption coefficient α and optical band gap (E_g)

The spectral distribution of the absorption coefficient α of the films was calculated from the relation $\alpha = 4\pi k/\lambda$, depend on the values of k calculated using Swanepoel's method. A plot of α as a function of photon energy hν is illustrated in Fig.6 and calculated values are given in Table 2.

Table 2. Optical parameters of $Se_{75}Te_{25-x}Cu_x$ thin films.

Samples	Optical band gap (Eg) in eV	Absorption coefficint (α) in cm^{-1}
$Se_{75}Te_{25}$	0.40	9.84 x10^{2}
$Se_{75}Te_{15}Cu_{10}$	0.23	1.30 x10^{3}

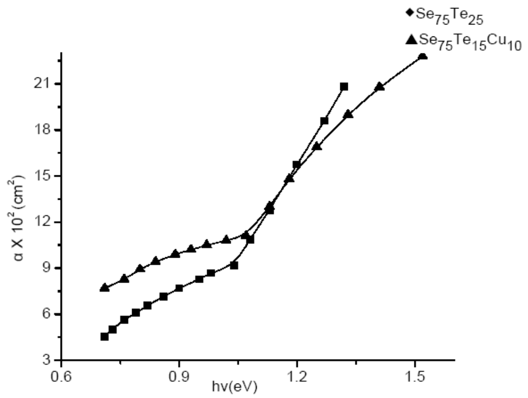

Fig. 6. Variation of absorption coefficient (α) vs photon energy (hν) for $Se_{75}Te_{25-x}Cu_x$.

The analysis of the absorption coefficient has been carried out to obtain the optical band gap E_g. The optical band gap has been estimated from absorption coefficient data as a function of wavelength by using Tauc Relation [20-22]

$$(\alpha \nu h)^{1/2} = A (h\nu - E_g) \qquad (11)$$

Where A is the edge width parameter representing the film quality, which is calculated from the linear part of this relation, E_g is the optical band gap of the material. The usual method for the determination of the value of E_g involves a plotting of $(\alpha h\nu)^{1/2}$ against hν as shown in Fig.7 and the values of E_g is given in Table.2 for the investigated samples. It is found that E_g decreases with Cu content. The Cu incorporation to $Se_{75}Te_{25}$ must bring about a compositional change of host material .The decrease in the optical band gap on addition of Cu in the present system may be due to the increase in disorderedness of the system and also increase in the density of localized states. This may be also correlated due to the shift in Fermi level. The Fermi energy depends upon the electron concentration, which is affected by the degree of disorderedness of the material. Due to these factors, distribution of electrons in the localized states changes consequently the position of Fermi level changes.

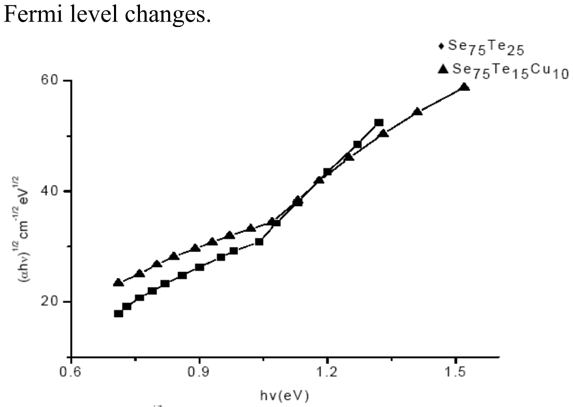

Fig. 7. Plots of $(\alpha h\nu)^{1/2}$ vs photon energy (hν) for $Se_{75}Te_{25-x}Cu_x$

4. Conclusion

The optical transmission spectra of thin films of $Se_{75}Te_{25-x}Cu_x$ (x = 0 & 10) are measured in the wavelength range 400-2100 nm by spectrophotometer. It is found that refractive index (n) decreases and extinction coefficient (k), absorption coefficient (α), imaginary dielectric constants (ε”) increases with Cu content. It is also observed that optical band gap decreases with Cu content. The decrease in band gap has been correlated with the increase in the density of localized states in the present glassy system.

Acknowledgements

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