

Effect of visible light on a-*SeTe* thin film

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The Se-Te alloy has more diverse scientific and practical applications in switching, memory devices, phase change recording devices etc as compared to a-Se, which crystallizes and ages easily. On illuminating the Se-Te thin film with visible light, it shows changes in structural, optical and electrical properties. This paper reports the changes in optical properties observed on illumination with electromagnetic radiation in visible region over Se-Te thin film. As a result of illumination, the increased absorption coefficient causes a decrease in the optical band gap. The change in the properties of thin film may be due to the increase in dangling bonds which increases the tailing in the band gap of the alloy.

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1. Introduction

Non-oxide chalcogenide glasses have attracted considerable scientific interest as a result of their exciting optical properties. Chalcogenide glasses are potential candidates for technological applications such as switching and memory devices, reversible phase change optical recordings, optical imaging and sensitive elements in various sensor systems [1–4].

Recently, studies on chalcogenide glasses and their thin films have attracted the attention of many researchers because of the challenging aspects such as the mechanism of radiation-induced phenomena. Apart from these, these glasses also exhibit many important properties like photodarkening [5], photobleaching [6], photodoping and photocrystallization [7]. Wide variety of changes in their structural properties, electronic transport properties and optical properties have been observed when they are exposed to light or heavy ion radiation [8–11]. The structure of chalcogenide glasses consists of a disordered network having some dangling bonds as defects. When these glasses are irradiated with heavy ions or light, bond breaking and bond rearrangement of atoms can take place, which results in the change in local structure of the amorphous network. These include subtle effects such as shifts in the absorption edge (photo-bleaching and photodarkening), and more substantial atomic and molecular reconfiguration such as photo-induced refractive index changes and photo-doping effects [7]. Generally, these phenomena are associated with the changes in the optical constants [12] and absorption edge shift [13], allowing the use of these materials in the fabrication of a large number of optical devices. This clearly underlines the importance of these glassy materials by accurate determination of their optical parameters. Hence these glasses offer a nice option for these technical applications by an accurate determination of various optical parameters.

Therefore, the authors have decided to investigate the optical and structural properties before and after the visible

light irradiation in *a-Se₈₅Te₁₅* thin film. An attempt has been made to analyze the change in optical parameters and structural characteristics of *a-Se₈₅Te₁₅* thin film on visible light irradiation. Swanepoel's method [14, 15] of using the transmission spectrum has been used for determining the optical constants.

2. Experimental details

Bulk alloy of *a-Se₈₅Te₁₅* is prepared by melt-quenching technique as described elsewhere [16]. The constituent elements taken are 5 N pure. Thin film of the said alloy is prepared by thermal evaporation technique in vacuum of 2×10^{-5} mbar on cleaned glass substrate. The absence of prominent peak in X-ray diffraction analysis confirmed the amorphous nature of the thin film (Figure 1).

The thin film is irradiated with visible light having intensity ≈ 8000 Lux in vacuum for 7 hours. The prominent peaks in X-ray diffraction analysis confirmed the phase change transition from amorphous to crystalline nature of the thin film (Fig. 1).

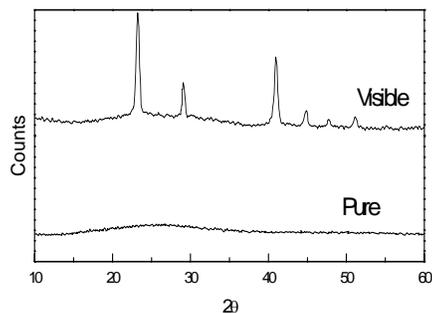


Fig. 1. X-ray diffraction of pure and visible light irradiated *a-Se₈₅Te₁₅* thin film.

The transmission spectra of the $a\text{-Se}_{85}\text{Te}_{15}$ thin film before and after the visible light irradiation have been measured by a double beam ultra violet-visible-near infrared (UV/VIS/NIR) spectrophotometer [Hitachi-330], in the transmission range of wavelength 400-2000 nm. The spectrophotometer was set with a suitable slit width of 1 nm, in the spectral range. All optical measurements have been performed at room temperature.

3. Theory

To analyse the change in optical properties of the visible light irradiated sample with respect to the pure thin film sample, Swanepoel's method has been used.

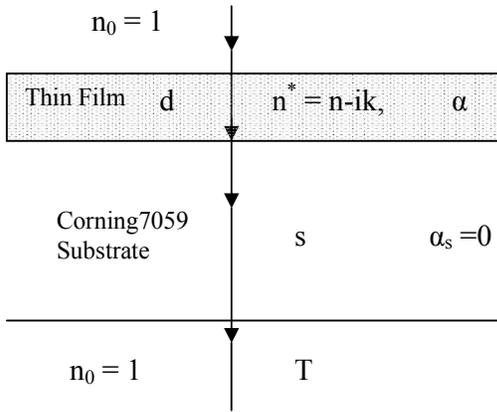


Fig. 2. System of an absorbing thin film on a thick finite transparent substrate.

The Swanepoel's method [14, 15] assumes that the sample is a thin film deposited on a transparent substrate having a refractive index 's'. The system is surrounded by air, whose refractive index is $n_0 = 1$ (Figure 2). The film has a complex refractive index $n^* = n - ik$, where n is the refractive index and k the extinction coefficient, which is related to the absorption coefficient (α) through the relation,

$$k = \alpha\lambda/4\pi.$$

The optical constants are obtained by using only the transmission spectrum. According to this method, which is based on the approach of Manifacier *et al.* [17], the refractive index in the region where $\alpha \approx 0$ is calculated by the following equation:

$$n = \sqrt{N + \sqrt{N^2 - S^2}} \quad (1)$$

where

$$N = 2s \frac{T_{\max} - T_{\min}}{T_{\max} T_{\min}} + \frac{s^2 + 1}{2} \quad (2)$$

T_{\max} and T_{\min} are the envelope values at the wavelengths in which the upper and lower envelopes and the experimental transmission spectrum are tangent

respectively. The accuracy to which λ can be measured is ± 1 nm. The maximum absolute accuracy of T_{\max} and T_{\min} is ± 0.001 . The values of n are calculated using Equation (1) at wavelengths corresponding to the tangent points.

If n_1 and n_2 are the refractive indices at two adjacent tangent points at λ_1 and λ_2 , then according to the basic equation for interference fringes

$$2nt = m\lambda \quad (3)$$

where m is an order number. The thickness is given by

$$t = \frac{\lambda_1 \lambda_2}{4(\lambda_1 n_2 - \lambda_2 n_1)} \quad (4)$$

It should be noted that owing to optical absorption, this particular equation is not valid at the interference maxima and minima, but is valid at the tangent points referred to [18]. Using equation (3), new more precise values of the refractive index and the film thickness were determined by a procedure which was explained in detail in [14,15].

The absorption coefficient (α) [15] can be calculated from the relation

$$x = \exp(-\alpha.t) \quad (5)$$

where x is absorbance, given by

$$x = \frac{E_M - \sqrt{E_M^2 - (n^2 - 1)^3(n^2 - s^4)}}{(n-1)^3(n-s^2)} \quad (6)$$

and

$$E_M = \frac{8n^2s}{T_{\max}} + (n^2 - 1)(n^2 - s^2) \quad (7)$$

In case of visible light irradiated thin film, there are no maxima and minima in the transmission spectrum. Therefore, from the transmission data, nearly at the fundamental absorption edge, the values of absorption coefficient (α) are calculated in the region of strong absorption using the relation

$$\alpha = \frac{1}{d} \ln\left(\frac{1}{T}\right) \quad (8)$$

The absorption coefficient of amorphous semiconductors in the strong-absorption region ($\alpha \geq 10^4 \text{ cm}^{-1}$), assuming parabolic valence and conduction band edges, is given by [18]

$$\alpha = \frac{B(\hbar\omega - E_g^{\text{opt}})^2}{(\hbar\omega)} \quad (9)$$

where $\hbar\omega$, E_g^{opt} and B , represent photon energy, optical gap and an energy independent constant, respectively.

Finally, the optical gap is calculated from the intersection of the plot of $(\alpha h\nu)^{1/2}$ vs. $h\nu$ with the abscissa axis.

4. Results and discussion

The thickness of thin film has been calculated by using equation (4). The thickness has been found to be ≈ 950 nm.

The transmission spectra of both the pure and the visible light irradiated thin film sample have been analysed to look for the changes in the band structure and optical parameters. The optical properties show a transition on subjecting the $a\text{-Se}_{85}\text{Te}_{15}$ thin film to visible light irradiation. Fig. 3 is a plot between percentage transmission and wavelength for pure and visible light irradiated thin film. The transmission in the irradiated thin film is very low (inset) as compared to pure film. This gives an indication of the crystalline state developed as a result of visible light exposure. The Scherrer [19-20] equation is used to calculate the crystallite or particle size

$$\beta_c = \frac{k\lambda}{D \cos \theta} \quad (10)$$

where D is particle diameter, 2θ is the diffraction angle, β_c is the full width at half maximum of the widened diffraction peak and k is a constant whose value depends upon particle shape and usually taken as unity. By using the above equation and diffraction peaks of the figure 1, the average particle size is ≈ 25 nm.

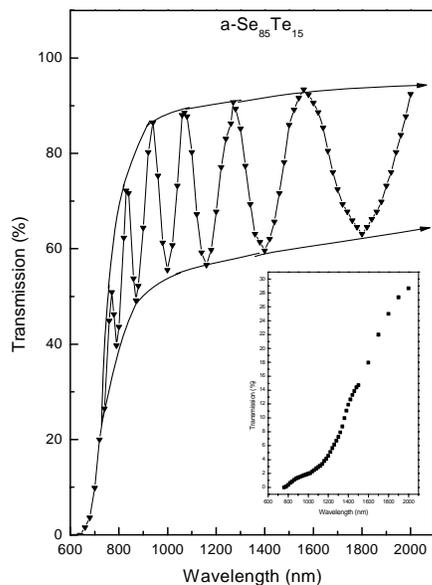


Fig. 3. Transmission spectrum of pure $a\text{-Se}_{85}\text{Te}_{15}$ thin film and that of visible light irradiated in inset.

The values of absorption coefficient (α) shows an increase with increase in the frequency of the incident radiation in both cases of pure and visible light irradiated

thin film. The absorption coefficient increases after the visible light irradiation as compared to the pure thin film. The optical energy gap (E_g^{opt}) is calculated by extrapolating the curve between $(\alpha h\nu)^{1/2}$ vs. $h\nu$ at the abscissa axis as shown in Fig. 4. The optical energy gap shows a decrease for the visible light irradiated thin film (inset), in its value from 1.40 to 1.23 eV. This decrease in the band gap may be due to an increase in the concentration of dangling bonds or surface voids on irradiating the $a\text{-Se}_{85}\text{Te}_{15}$ thin film sample with visible light. In other words, this implies an increase in the density of the surface voids of the thin film. The crystallised film developed due to the visible light irradiation changes to micro and nano crystallites with progress in visible radiation exposure on the thin film. Due to the transition from amorphous to crystalline state, the tailing of the conduction and valence band is increased. This causes a decrease in the optical band gap.

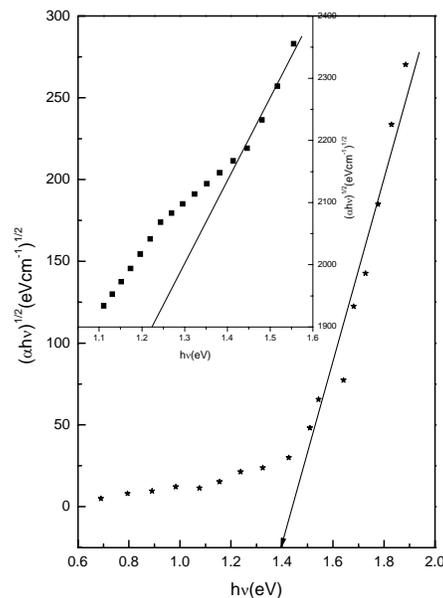


Fig. 4. Plot of $(\alpha h\nu)^{1/2}$ vs. $h\nu$ for pure $a\text{-Se}_{85}\text{Te}_{15}$ thin film and visible light irradiated in inset.

There may be an increase in disorder at the expense of delocalized states near the band edges.

5. Conclusions

The optical properties of $a\text{-Se}_{85}\text{Te}_{15}$ thin film on visible light irradiation show a characteristic change. The optical energy gap E_g^{opt} decreases and the absorption coefficient (α) increases on visible light irradiation. The film undergoes crystallization with average particle size is ≈ 25 nm. This indicates an ordering of the bonds in thin film sample on visible light irradiation. This may be due to the enhanced valence band tailing on visible light irradiation.

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