JOURNAL OF OPTOELECTRONICS AND ADVANCED MATERIALS Vol. 9, No. 10, October 2007, p. 3097 - 3099

Phase transition in Se-Te thin film on UV illumination

V. SHARMA*, A. THAKUR[a]
Jaypee University of Information Technology, Waknaghat, Solan – 173 215, India
[a]University College of Engineering, Punjabi University, Patiala-147 002, India

The *Se-Te* glassy alloy presents an interesting alternative with respect to application point of view. These alloys are more advantageous as compared to *a-Se*. The alloy witnesses different changes in its structural, optical and electrical properties on treating it with electromagnetic radiation. This gives an important method to investigate the different possibilities of applications of these materials like switching, memory devices, phase change recording devices etc. The present paper reports such changes observed on exposing the $a\text{-}Se_{85}Te_{15}$ thin film deposited by vacuum evaporation technique. The optical band gap of the alloy decreases on exposing the thin film to UV radiation. The absorption coefficient of the illuminated thin film shows an increase. The structural study of the thin films indicates a clear transition from amorphous to nano-crystallite structure.

(Received July 3, 2007; accepted October 1, 2007)

Keywords: Se-Te amorphous film, Phase transition, UV irradiation

1. Introduction

Chalcogenide glasses are of interest for applications in infrared technology, including the fabrication of optical elements such as mirrors and filters. The low characteristic vibrational frequencies of chalcogenide bonds allow them to transmit far out into the infrared region [1]. Amorphous chalcogenide semiconducting materials undergo various transformations upon photoexcitation [2]. Generally, it is believed that the photoinstability is a privilege of the amorphous state and is due mainly to a rearrangement in the local order of the glassy network [3]. These glasses show a variety of photo-stimulated phenomena when exposed to light or other radiations [4,5]. On irradiating these glasses with high energy particles or light, bond breaking and bond rearrangement can takes place, which results in the change of local structure of the glassy materials. These include subtle effects such as shifts in the absorption edge (photo-bleaching and photo-darkening), and more substantial atomic and molecular reconfiguration such as photo-induced refractive index changes and photo-doping effects [6]. Generally, these phenomena are associated with the changes in the optical constants [7] and absorption edge shift [8], 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 change in optical and structural properties before and after the UV irradiation in $a\text{-}Se_{85}Te_{15}$ thin film. An attempt has been made to analyze the change in optical parameters and structural characteristics of $a\text{-}Se_{85}Te_{15}$ thin film on UV irradiation. Swanepoel's method [9,10] of using the transmission spectrum has been used for determining the optical constants.

2. Experimental procedure

Glassy alloy of $a\text{-}Se_{85}Te_{15}$ is prepared by quenching technique as described elsewhere [11]. Thin film of the alloy is prepared by vacuum evaporation technique on well-degassed Corning 7059 glass substrate at room temperature and base pressure of ~ 2×10^{-5} mbar using a molybdenum boat. Amorphous nature of the sample has been confirmed by X-ray diffraction technique. No prominent peak has been observed in the thin film (Fig. 1).

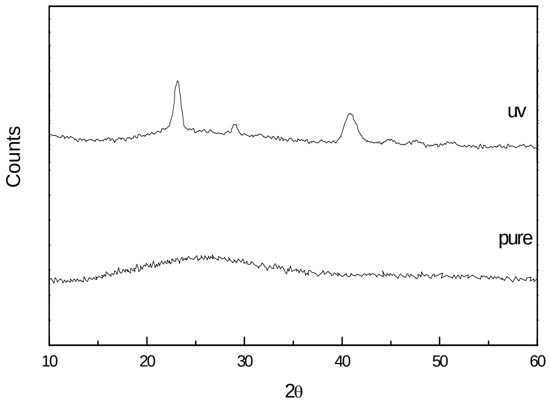

Fig. 1. X-Ray Diffraction of Pure and UV irradiated $a\text{-}Se_{85}Te_{15}$ thin film.

The thin film is irradiated at room temperature in vacuum (~ 10^{-3} mbar), with UV light source having light intensity ~ 8000 Lux for 7 hours. The normal incidence transmission spectra of the substrate with and without $a\text{-}Se_{85}Te_{15}$ thin film have been measured by a double beam UV/VIS/NIR computer controlled spectrophotometer [Hitachi-330], in the transmission range 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 (300 K).

3. Theory

The model behind Swanepoel's method [9,10] assumes that the sample is a thin film of non-uniform thickness deposited on a transparent substrate having a refractive index 's'. The system is surrounded by air, whose refractive index is $n_0 = 1$. The film has a complex refractive index $n^* = n - i\,k$, 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.* [12], the refractive index in the region where $\alpha \approx 0$ is calculated by the following equation:

$$n = \sqrt{N + \sqrt{N^2 - S^2}} \tag{1}$$

where

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

$T_{\max}$ and $T_{\min}$ are the envelope values at the wavelengths in which the upper and lower envelops and the experimental transmission spectrum are tangent respectively, as shown in Fig. 2. 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

$$2nt = m\lambda \tag{3}$$

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

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

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 [9]. 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 [9,10].

The absorption coefficient (α) [10] can be calculated from the relation

$$x = \exp(-\alpha . t) \tag{5}$$

where *x* is absorbance, given by

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

and

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

In case of UV irradiated thin film there is 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

$$\alpha = \frac{1}{t}\ln\left(\frac{1}{T}\right) \tag{8}$$

The absorption coefficient of amorphous semiconductors in the strong-absorption region ($\alpha \geq 10^4$ cm^{-1}), assuming parabolic valence and conduction band edges, is given by [13]

$$\alpha = \frac{B\left(\hbar\omega - E_g^{opt}\right)^2}{(\hbar\omega)} \tag{9}$$

where ħω, 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 $(\alpha\hbar\omega)^{1/2}$ vs. ħω with the abscissa axis.

4. Results and discussion

Thickness (t) of thin film is calculated by using equation (4) and it is ~ 900 nm. X-ray diffraction studies are carried out in order to get an idea about structural changes produced in *a*-$Se_{85}Te_{15}$ thin film by UV irradiation. It is evident from Fig. 1 that *a*-$Se_{85}Te_{15}$ thin film undergoes amorphous to crystalline transition as a result of UV irradiation. The increase in sharpness of peaks may be attributed to the fact that *a*-$Se_{85}Te_{15}$ has undergone a transition to crystalline state to a certain extent as a result of UV treatment, and thereby a long range periodic rearrangement of atoms is achieved. These types of changes on heat treatment have also been reported by Biswas *et al.* [14].

The Scherrer [15,16] equation is used to calculate the crystallite or particle size

$$\beta_c = \frac{k\lambda}{D\cos\theta} \tag{10}$$

where D 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 ≈ 12 nm.

Fig. 2 is a plot between percentage transmission and wavelength for pure and UV irradiated thin film. From Fig. 2 it is clear that the transmission in the UV irradiated thin film is very low as compared to pure film. This also indicates that there is crystallization due to UV irradiation.

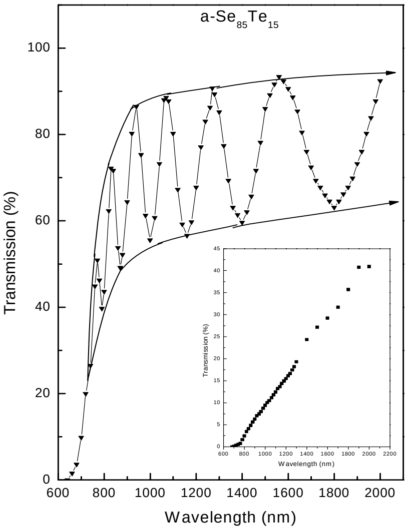

Fig. 2. Optical transmission spectrum, T(λ) for Pure a-Se$_{85}$Te$_{15}$ thin film. Inset: UV irradiated thin film.

The values of absorption coefficient (α) are increased with increase in the photon energy for pure and UV irradiated thin film. The values of absorption coefficient are increased after the UV irradiation. Finally, the optical gap (E_g^{opt}) is calculated from the intersection of the plot $(\alpha h\nu)^{1/2}$ vs. hν with the abscissa axis. The value of E_g^{opt} decreases from (1.40 ± 0.01) to (1.30 ± 0.01) eV. This decrease in the band gap is explained by considering an increase in the dangling bonds or surface voids on UV irradiation of the *a-Se$_{85}$Te$_{15}$* thin film. There is development of nanophases in the structure of thin film upon irradiation. Due to this the extent of tailing is increased and band gap is decreased. There may be an upward shift in the top of the valence band edge and increase in disorder at the expense of delocalized states near the band edges [17].

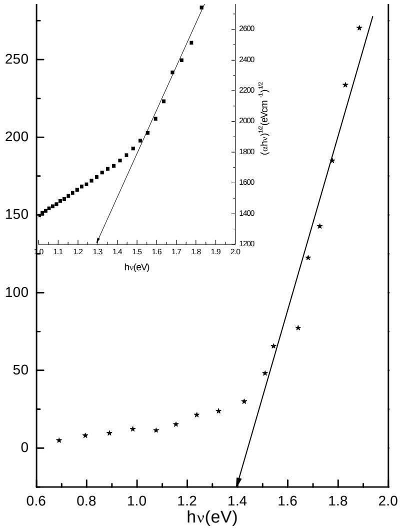

Fig. 3. Plot of $(\alpha h\nu)^{1/2}$ vs. hν for pure a-Se$_{85}$Te$_{15}$ thin film . Inset: UV irradiated thin film.

5. Conclusions

The irradiation of *a-Se$_{85}$Te$_{15}$* thin film with UV radiation has pronounced effect on the optical and structural properties. There is decrease of E_g^{opt} with UV irradiation in the thin film. The film undergoes crystallization with particle size ~ 12 nm. The absorption coefficient (α) increases on UV irradiation. The results have been explained on the basis of enhanced valence band tailing caused by UV irradiation.

Acknowledgements

The authors acknowledge the Centre of Advanced Study in Physics and RSIC, Panjab University Chandigarh-160014, India for various experimental measurements.

References

[1] P. J. S. Ewen, C. W. Shinger, A. Zakery, A. Zekak, A. E. Owen, SPIE Infrared Optoelectron. Mater Dev. **1512**, 101 (1991).
[2] DeNeufville J. P. In: Seraphin B. O., editor. Optical properties of solids-new developments. Amsterdam: North Holland, 1975. p. 437.
[3] K. Tanaka, In: F. Yonezawa, editor. Fundamental physics of amorphous semiconductors Berlin: Springer, 1981, p. 104.
[4] A. Arsh, M. Klebanov, V. Lyubin, L. Shapiro, A. Feigel, M. Veinger, B. Sfez, Optical Mat. **26**, 301 (2004).
[5] V. Lyubin, M. Klebanov, A. Feigel, B. Sfez, J. Non-Cryst. Solids **459,** 183 (2004).
[6] M. Mitkova, M. N. Kozicki, H. C. Kim, T. L. Alford, J. Non-Cryst. Solids **338-340**, 552 (2004).
[7] E. Marquez, T. Wagner, J. M. Gonzalez-Leal, A. M. Bernal-Oliva, R. Prieto-Alcon, R. Jimenez-Garay, P. J. S. Ewen, J. Non-Cryst. Solids **274**, 62 (2000).
[8] V. M. Lyubin, M. Klebanov, B. Safe, B. Ashkinadze, Mat. Lett. **58**, 1706 (2004).
[9] R. Swanepoel, J. Phys. E: Sci. Instrum. **17**, 896 (1984).
[10] R. Swanepoel, J. Phys. E **16**, 1214 (1983).
[11] A. Thakur. P. S. Chandel, V. Sharma, N. Goyal, G. S. S. Saini, S. K. Tripathi**,** J. Optoelectron. Adv. Mater. **5**, 1203 (2003).
[12] J. C. Manifacier, J. Gasiot, J. P. Fillard, J. Phys. E: Sci. Instrum. **9**, 1002 (1976).
[13] J. Tauc, J. Non-Cryst. Solids **8**, 569 (1972).
[14] S. K. Biswas, S. Chaudhury, Phys. Status Solidi A **105**, 407 (1988).
[15] P. Scherrer, Math. Phys. K **1**, 98 (1918).
[16] Al. L. Efros, A. L. Efros, Sov. Phys. Semicon. **16**, 772 (1982).
[17] L. Tichy, H. Ticha, P. Nagels, R. Callaerts, J. Non-Cryst. Solids **240**, 177 (2000).

---

[*] Corresponding author: vneetsharma@gmail.com