ISSN : 0974 - 7524 Volume 8 Issue 2

Trade Science Inc.

Physical CHEMISTRY
An Indian Journal

Full Paper

PCAIJ, 8(2), 2013 [54-58]

Optical parameters of amorphous selenium deposited by thermal evaporation technique

Nadir F.Habubi[1]*, Nabeel A.Bakr[2], Sabah A.Salman[2]

[1]Department of Physics, College of Education, Al-Mustansiriyah University, Baghdad (IRAQ)

[2]Department of Physics, College of Science, University of Diyala, Diyala, (IRAQ)

E-mail : nadirfadhil@yahoo.com

PACS: 78.20.-e, 78.20.Ci, 78.40.Fy

ABSTRACT

Thin films of amorphous selenium have been prepared by thermal evaporation technique. The analysis proposed by Swanepoel has been successfully employed to determine the average thickness and refractive index of the films with high accuracy in the spectral range of 540-1050 nm. The absorption coefficient α, therefore extinction coefficient k, have been determined from the transmission spectra at the strong absorption region. The optical absorption edge is described using Tauc formula and it has been found that the transition was direct with an energy gap equal to 2.02 eV. The dispersion of the refractive index is discussed in terms of the single-oscillator Wemple–DiDomenico model. The dispersion energy E_d and single-oscillator energy E_o were found to be 3.888 eV and 25.514 eV respectively.

KEYWORDS

Thin films;
Optical properties;
A-selenium;
Swanepoel method;
Thermal evaporation;
Tacu model.

INTRODUCTION

In recent years many efforts have been subjected for the study for the most commercial important chalcogenide semiconductor, the amorphous selenium, which has been known as one of the important semiconductors that exhibits photoconductivity, low photomelting temperature and switching phenomenon[1-4]. Amorphous selenium is essentially a glass, and all glasses exhibit some degree of structural relaxation effects during which the physical properties such as the refractive index and the band gap change with time which is called aging. Selenium has been used in many applications such as electrophotography photoinduced anisotropy, photoconductive devices, photovoltaic, rectifiers, photocells and many more devices[5-11].

There are many research papers that concern the development of Se thin films and their functional properties[12-14], their optical properties are known to be strongly depend on the preparation technique, so thermal evaporation method was adopted to fabricate a-Se thin film.

In this paper, a fast and nondestructive technique was used to determine the optical constants of amorphous selenium in order to obtain its response to the incident electromagnetic radiation in the visible region.

EXPERIMENTAL

High quality selenium obtained from the (BDH

chemicals Ltd England) was deposited by thermal evaporation technique. The glass substrates were cleaned with detergent, degreased with trichloroethylene, acetone and rinsed with deionized water in an ultrasonic cleaner. A rectangular molybdenum boat of (2895 k) melting point was used as the evaporation source. High vacuum unit (Edwards coating unit model 306 A) was used in the preparation of Se thin film, at a glass substrate of 300 k. The substrate was fixed on a spherical holder and placed at a height of 15 cm above the boat. The vacuum was maintained at 10^{-5} mbar and the deposition rate was kept at 10Å/sec in order to obtain Se thin films with high homogeneity. The optical transmission spectrum for the deposited thin films were recorded using UV-VIS double beam spectrophotometer (schimadzu 1650 Japan) in the wavelength range of 540-1050 nm.

RESULTS AND DISCUSSION

Optical parameters of the films were calculated from the transmission spectra using Swanepoel's method[15,16]. Figure 1 shows typical transmission spectra for the investigated films. Interference maxima and minima due to multiple reflections on the film surface can be observed.

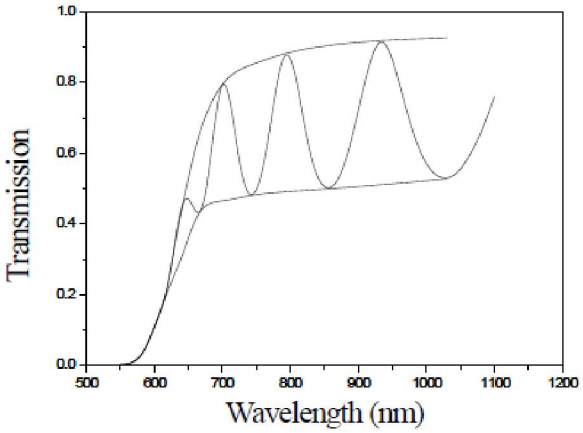

Figure 1 : Transmission spectrum for amorphous selenium thin film

The index of refraction at different wavelengths was calculated using the envelope curve for T_{max} and T_{min} in the transmission spectra. This relation can be expressed as follows:

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

where

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

n_s is the refractive index of the substrate (in our case n_s was considered to be constant and equal to 1.533 for the glass substrate). The values of refractive index as calculated from equation (1) are shown in TABLE 1.

The thickness of the thin film d can be calculated by knowing the values of refractive indices n_1 and n_2 at two adjacent maxima and minima corresponding to their wavelength λ_1 and λ_2, and the thickness is given by:

$$d = \frac{\lambda_1 \lambda_2}{2(\lambda_1 \lambda_2 - \lambda_2 \lambda_1)} \quad (3)$$

The values of d determined by this equation are listed as d_1 in TABLE 1. The average value of $\overline{d_1}$ is 800.25 nm. This value can be used with n to calculate m_o according to the following equation:

$$2nd = m_o \lambda \quad (4)$$

where m_o is an integer for maxima and half integer of minima. The accuracy of d can be significantly increased by taking the corresponding exact integer or half integer values of m associated to each extreme point, and deriving a new thickness d_2 from equation (4). The values of d_2 found in this way have a smaller dispersion and the average value of d_2 are $\overline{d_2}$ is 804.35 nm. With the precise values of m and d, equation (4) was used again to get the values of n_2 at each wavelength, thus the final values of the refractive index are obtained. All the calculated values are listed in TABLE 1. Figure 2 shows the refractive index versus wavelength, and it can be seen that n decreases with the increase in wavelength and this may be correlated with the increase in transmittance and decrease in absorbance. The decrease in the value of refractive index with wavelength shows the normal dispersion behavior of the material.

Now the values of n_2 can be fitted using Sellmeier equation which is represented by the following relation:

$$n^2 = A + \frac{B\lambda^2}{\lambda^2 - C} \quad (5)$$

Where A,B and C are constants. By solving this equation, the values of A, B and C were found to be as 7.12061, 0.86286 and 2.97664 x 10^5 respectively.

Full Paper

These values were used in equation (5) to calculate the values of refractive index for all the investigated wavelengths. Knowing n and d, the absorption coefficient and the extinction coefficient can be obtained by using the following formula:

$$x = \frac{\left(E_M[E_M^2 - (n^2-1)^2(n^2-n_s^4)]^{1/2}\right)}{(n-1)^s(n-n_s^2)} \quad (6)$$

where,

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

The absorption coefficient α is calculated from the equation[18]:

$$\alpha = \frac{1}{d} ln \frac{1}{x} \quad (8)$$

Figure 3 depicts the variation of absorption coefficient with wavelength. It can be seen that the value of α decreases exponentially as the wavelength increases and then become nearly constant in the wavelength range of

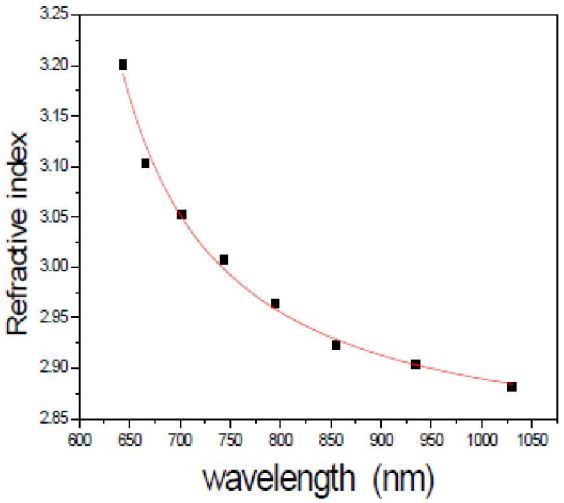

Figure 2 : Refractive index versus wavelength for amorphous selenium thin film

710-1050 nm.

The optical absorption edge was analyzed by Tauc method using the following equation[19]:

$$\alpha = \frac{B(h\nu - E_g)^{1/2}}{h\nu} \quad (9)$$

where $h\upsilon$ is the incident photon energy, B is a constant which is a measure of the extent of band tailing and E_g is the forbidden energy gap. The linear dependence of $(\alpha h\upsilon)^2$ on in the high absorption region for amorphous Se films is shown in Figure 4 which indicates the presence of direct transition between the parabolic edges of the valance and conduction bands. The extrapolation of the linear portion of the plot on to the photon energy axis determines the energy band gap of the film which was found to be 2.02 eV. The extinction coefficient k is calculated using the following relation[20]:

$$k = \frac{\alpha\lambda}{4\pi} \quad (10)$$

Figure 5 shows the variation of the extinction coefficient with wavelength. It is clearly seen that the value of k decreases sharply in the visible region, and starts to increase in the near infrared region. The decrease in the values of k with increasing the wavelength shows that in the visible region the fraction of light lost is due to

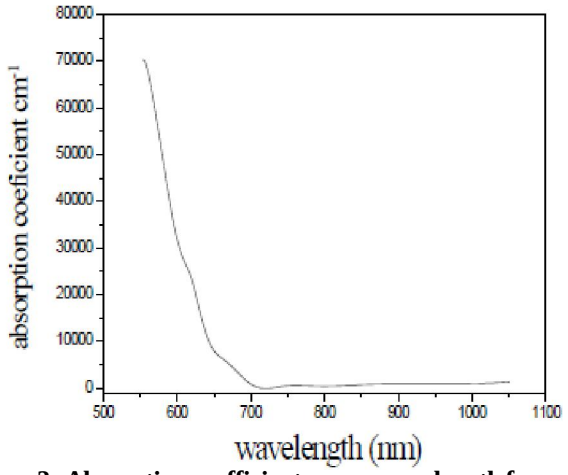

Figure 3 : Absorption coefficient versus wavelength for amorphous selenium thin film

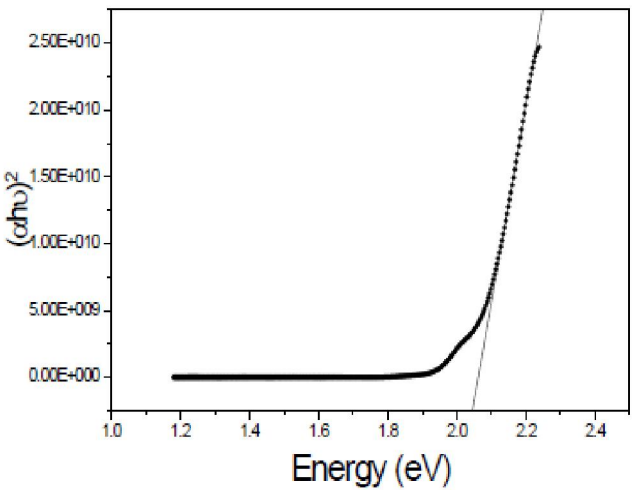

Figure 4 : $(\alpha h\nu)^2$ versus photon energy of the amorphous selenium thin film

scattering and absorbance decrease.

The real and imaginary parts of dielectric constant

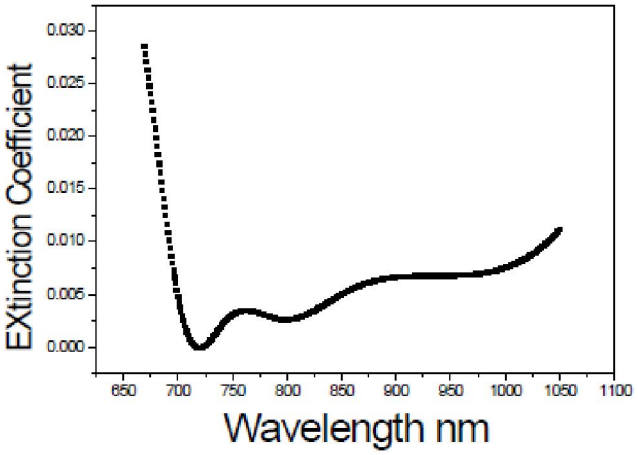

Figure 5 : Extinction coefficient versus wavelength for amorphous selenium thin film

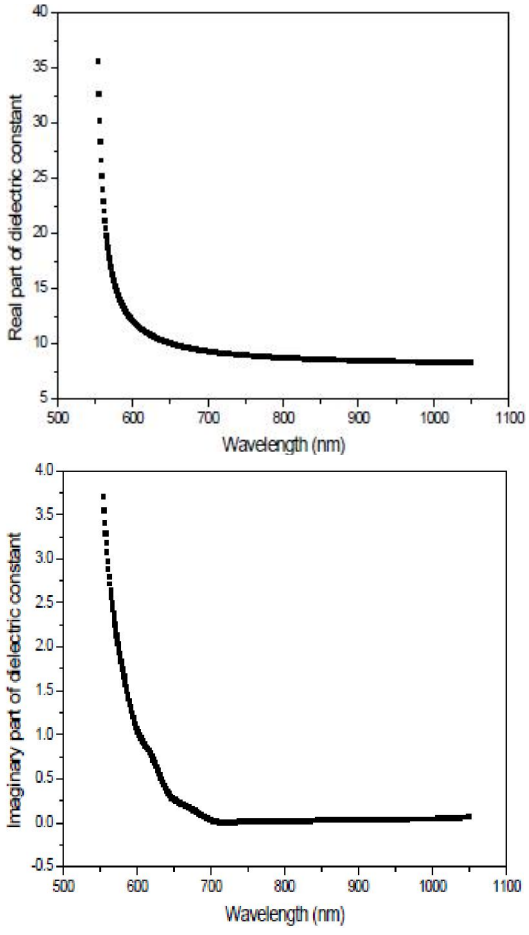

Figure 6 : Real and imaginary parts of the dielectric constant versus wavelength for amorphous selenium thin film

can be calculated using the following relations[21]:

$$\varepsilon_1 = n^2 - k^2 \quad (11)$$

$$\varepsilon_r = nnk \quad (12)$$

Figure 6 shows the real and imaginary parts of the dielectric constant versus wavelength. The real part describes the propagation characteristics (velocity v = ω / *k'*) while the imaginary part describes the rate of attenuation along the propagation direction. Both could be used to define the refractive index of the medium (film material) and the absorption coefficient. It can be seen that the real part of the dielectric constant decreases with increasing wavelength in the visible region while their values remain approximately constant in the near infra-red region. The real and imaginary parts follow the same pattern and the values of the real part are higher than the imaginary part.

In order to analyze the refractive index dispersion of the films, we used the single-oscillator model developed by DiDomenico and Wemple. The refractive index at can be expressed in terms of the dispersion energy E_d and single-oscillator energy E_o. The single-oscillator model for the refractive index dispersion is expressed as follows[22]:

$$n^2 = 1 + \frac{E_d E_0}{E_0^2 - (h\nu)^2} \quad (13)$$

Plotting $(n^2 - 1)^{-1}$ versus as shown in Figure 7, allows us to determine the oscillator parameters. Eo and Ed values were calculated from the slope and intercept on the vertical axis of $v(n^2 - 1)^{-1}$ versus plot. The E_o and E_d values are found to be 3.888 eV and 25.514 eV respectively. E_o, is an average energy gap and can be related to the

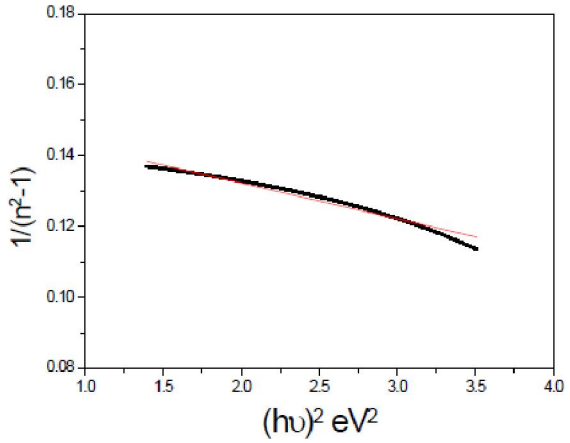

Figure 7 : $(n^2 - 1)^{-1}$ versus $(hv)^2$ for amorphous selenium thin film

band gap, Eg, in close approximation $E_0 \approx 2Eg$[23]. The obtained values of energy band gap is E_g=1.9 eV.

Full Paper

CONCLUSIONS

The optical characterization of thermally evaporated of amorphous Se semiconducting films has been carried out using only the transmission spectrum at normal incidence. The envelope method suggested by Swanepoel has been successfully applied to the films with higher thickness, with a reasonable number of interference fringes. The results indicate that the values of n are 2.8812-3.2006 The optical band gap was appropriately fitted to the direct transition model proposed by Tauc in the strong-absorption region of investigated films and its value was 2.02 eV. The value of the band gap is compared with its value obtained by the method proposed by wimple –DiDomenico and was found to be 1.9 eV.

TABLE 1 : The calculated parameters due to swanepoel method for amorphous selenium thin films

Λ	T_{max}	T_{min}	n	d_1	m_o	m	d_2	n_2
643.6	0.518	0.316	3.27070		8.130	8.0	787.1	3.2006
665.7	0.654	0.394	3.04700		7.330	7.5	819.3	3.1036
701.6	0.845	0.453	3.06250	697.5	6.980	7.0	801.8	3.0529
744.3	0.885	0.473	3.02120	965.2	6.496	6.5	800.7	3.0074
794.6	0.910	0.500	2.93300	742.0	5.910	6.0	812.8	2.9636
855.0	0.916	0.492	2.97552	863.6	5.570	5.5	790.2	2.9232
934.4	0.927	0.515	2.89153	838.0	4.950	5.0	807.9	2.8812
1030.0	0.931	0.528	2.84370	695.2	4.420	4.5	815.0	2.8812

REFERENCES

[1] A.Solieman, A.A.Abu-Sehly; Modeling of optical properties of amorphous selenium thin film. Physica B, **405**, 1101-1107 **(2010)**.

[2] L.I.Berger; Semiconductor materials. CRC Press, Boca Raton, FL, **(1997)**.

[3] V.V.Poborchii, A.V.Kolobov, K.Tanaka; Appl.Phys. Lett., **74**, 215 **(1999)**.

[4] B.Gates, B.Mayers, B.Cattle, Y.Xia; Adv.Funct. Mater., **12**, 219 **(2002)**.

[5] J.C.Chou, S.Y.Yang, Mater.Chem.Phys., **78**, 666 **(2003)**.

[6] JR.A.C.M.M.Van Swaaij, W.P.M.Willems, J.P.Lohher, J.Bezemer, W.F.Van der Weg; J.Appl. Phys., **77**, 1635 **(1995)**.

[7] V.G.Zhdanov, B.T.Kolomiets, V.M.Lyubin, V.K.Malinovsky; Phys.Status Solidi A, **52**, 621 **(1979)**.

[8] R.Roy, V.S.Choudhary, M.K.Patre, A.Pandya; J.of Optoelectronics and Advanced Materials, **8**, 1352 **(2006)**.

[9] S.O.Kasap, J.A.Rowlands; J.Mater.Electron., **11**, 179 **(2000)**.

[10] W.Ahao, D.C.Hunt, T.Kenkichi m, J.A.Rowlands; Nucl.Instrum.Meth.Phys.Res.A, **549**, 205 **(2005)**.

[11] K.Tanaka, A.Odajima; Solid State Commun., **43**, 621 **(1982)**.

[12] K.D.Almeida, K.Napo, G.Safoula, S.O.Djobo, J.C. Bernede; J.Mater.Sci., **35**, 2985 **(2000)**.

[13] K.Bindu, M.Lakshmi, S.Bini, C.S.Kartha, K.P.Vijaykumar, T.Abe, Y.Kashiwaba; Semicond. Sci.Technol., **17**, 270 **(2002)**.

[14] M.M.Abdul, G.M.A.Al, B.K.A.Wishah; International J.Electron., **85**, 21 **(1998)**.

[15] R.Swanepoel; J.Phys.E:Sci.Instrum., **16**, 1214 **(1983)**.

[16] R.Swanepoel; J.Phys.E:Sci.Instrum., **17**, 896 **(1984)**.

[17] J.W.Mares, M.Falanga, W.R.Folks, G.Boreman, A.Osinsky, B.Hertog, J.Q.Xie, W.V.Schoenfeld; Journal of Electronic Materials, **37(11)**, 1665 **(2008)**.

[18] P.Sharma, S.C.Katyal; J.Phys.D: Appl.Phys., **40**, 2115 **(2007)**.

[19] J.Tauc, A.Menth; J.Non-Cryst.Solids, **8-10**, 569 **(1972)**.

[20] D.C.Sati, R.Kumar, R.M.Mehr; Taurk J.Phys., **30**, 519 **(2006)**.

[21] F.A.Jenkins, H.E.White; Fundamentals of optics, 4th Edition, McGraw Hill: New York, **(1976)**.

[22] M.DiDomenico, S.H.Wemple, J.Appl.Phys., **40**, 720 **(1969)**.

[23] R.Pietro-Alcon, J.M.Gonzalez-Leal, R.Jimenez-Garay, E.Marquez, J.Optoelectron.Adv.Mater., **3**, 287 **(2001)**.