CALCULATE THE VALUES OF SOME PHYSICAL PROPERTIES OF $Se_{0.3}Te_{0.7}$ ALLOY PREPARED AT DIFFERENT SUBSTRATE TEMPERATURES

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Abstract

In this paper; $Se_{0.3}Te_{0.7}$ alloy was prepared by mixing Selenium and tellurium of high purity using vacuum evaporation technique, this alloy was prepared as thin films at different substrate temperature; (25, 50, 100, 150) C^o. The annealing was done for some of the prepared films at 200 ^oC.

The powder of the prepared alloy was tested by X-Ray diffraction; the result shows that the structure of the $Se_{0.3}Te_{0.7}$ alloy was polycrystalline.

From Hall effect results; the films was found as p-type, the density of the charge carriers (N) was calculated at different substrate temperature, the concentration of charges carriers of the annealed films was decreased.

The optical properties of $Se_{0.3}Te_{0.7}$ films were studied, the values of the optical energy gaps were calculated and it was 0.48 eV at room temperature, this value was increase at the increasing of the substrate temperature. The value of energy gap of the annealed film was calculated and it was 0.62 eV at room temperature.

The refraction index was calculated at room temperature as a function of the wave length at 2100 nm; it found to be 4.2.

Introduction

The researches interest about the application SeTe alloys because it is widely using in high power laser diodes and irreversible phase change optical recorder [1].

Thin films are uses in many develop technical applications and used for manufacturing the infrared detection and low cost solar cell, therefore it is very important to study the electrical and the optical properties of the film [2, 3]

SeTe films is important compound because it is isomorphous and it has low fluidity point and high vapors pressure in optical record medic therefore many researches were prepared this alloy as a thin films [4, 5].

Selenium and Trillium elements have same hexagonal crystal structure, Nodaetal [6] prepared SeTe alloy, he found that the deposit $Se_{1-}xTex$ film on glass substrate under vacuum at room temperature will be polycrystalline at X>0.25. Walanabe and Kao [7] found that part of the prepared $Se_{1-}xTex$ films, which deposit under vacuum at room temperature, for x value between 0.5-0.6 will be polycrystalline and other parts is amorphous.

lanyon [8] found that the deposited SeTe films under vacuum at room temperature is amorphous and it is convert to polycrystalline during the annealing management.

Motand Davis [9] explains the reason structure conversion from amorphous state to polycrystalline state during increasing of the concentration of Te in SeTe alloys. Tellurium element considered as stimulator pole factor so the existence of Te in a chain of Se-Te may be supporting by thermal-dissociation process that made the Se-Te bond weaker then Se-Se bond and this will make the crystalline structure easy.

The optical properties of SeTe films were studied to know the changing of the energy gap of the compound directly, the spectrum area that is near the absorption edge considered to be very important for the study of the optical energy gap and electronic levels properties [8].

The values of energy gap (E_g) of SeTe alloy depend on its structure and on the method of preparing alloy. Daware et al [10] found that the energy gap of the crystalline-Trillium (c-Te) and

the amorphous-Trillium (a-Te) is ranging between (0.5-0.8) eV respectively, while the amorphous Selenium have energy gap between (1.86-2.2) eV [7, 10, 11], the optical absorption edge for the amorphous Se and Te move toward high energies in comparative with crystal Te and Se.

The optical absorption in semiconductor happened when the incident photon has enough energy to stimulate the electrons from the top of the equivalent band to the bottom of the conduction band. The theory of the optical absorption gives the relationship between the absorption coefficient (α) and the incident photon energy hν, for direct allowed transition:

$$\alpha = (h\nu - E_g)^r \quad \text{..... (1)}$$

h is plank constant; ν is frequency of the incident photon; hν is the energy of incident photon, r is constant which takes the values (1/2, 3/2, 2, 3) depending on the material and the type of the optical transition whether it is direct or indirect [12].

There are many important parameters must study to calculate the absorption coefficient; the intensity of the incident light, the nature and the thickness of the material. The amount of light that transmitted through thin film material depends on the amount of the reflection and absorption that takes place along the light path [13].

If the intensity of the incident light on material of thickness (d) is (I_o), the intensity of the penetrated light (I) through this thickness gives by this relation:

$$I = I_o \exp(-\alpha d) \quad \text{.....(2)}$$

$I\backslash I_o$; this ratio named the penetration T_λ.

The absorption A_λ can be calculates from the equation:

$A_\lambda = \log 10 / T_\lambda$

$T_\lambda = \exp[-2.303 A_\lambda]$

$A_\lambda = \log 10\ I_O/I$

$$\alpha = 2.303\ A_\lambda / d \quad \text{.....(3)}$$

The absorption coefficient α can be calculated from equation (3) as a function of wavelength.

From measurement of the energy of incident photon and the absorption coefficient; the value of the energy gap can be calculated by using equation (1) at the extension of liner part of the curve to hν = 0 (at x-axis).

Hall coefficient can be calculated by studying the Hall Effect, this studying is important to find the concentration and type of charge carriers from equation [14]:

$$R_H = \frac{\nu_H}{I} \cdot \frac{d}{B} \quad \text{.....(4)}$$

B=the intensity of magnetic field.

d=the film thickness.

R_H=Hall coefficient, V_H = Hall Voltage

$$R_H = -1\backslash Ne \quad \text{.....(5)}$$

N=concentration ratio of charge carriers

e= charge of electron

For semiconductor type n, Hall coefficient (R_H) will be negative but in semiconductor type p R_H will be positive.

The concentration of charge carriers for p-type increase with increasing of deposition rate and may be reach to 2×10^{18} cm^{-3} at using high deposition rate (50 A^oS^{-1}) also the concentration of charge carriers increase with the increases of the film thickness [15, 16].

The optical constants of SeTe were studied by many researchers, Dawar et. al [10] study the optical properties of $Se_{1-X}Te_X$ films at ($0<x<1$), depending on the reflectance and the transmittance measurement among the range of wave lengths (400-2500) nm. Dawar et al calculate the values of the refractive index (n) for Se and Te films, it was 2.8, 6.6 respectively.

The optical constants of the amorphous $Se_{1-X}Te_X$ films at ($0<x<0.4$) were studied by Adachiet et al [11] depending on transmittance measurement (T) among the range of wave lengths (350-2500) nm by using the relation between the refraction index (n) and the extinction coefficient (k) for the compound N:

$N = n - i\,k = \sqrt{€}$

€ is the dielectric constant of compound

$€ = €_1 + €_2$

$$n = 1.13\ X + 3.04 \quad \text{.....(6)}$$

The real and the imaginary dielectric constant is given by using the value of k:

$k = 2.1X + 0.55$

$$€_1 = n_2 - k_2,\ €_2 = 2nk \quad \text{.....(7)}$$

$€_1$= real dielectric constant, $€_2$=the imaginary dielectric constant.

The experiential work

Selenium (Se) and Tellurium (Te).powder elements of high purity (99.99%) and high precision weights were used to prepare $Se_{0.3}Te_{0.7}$ alloy. 1.149($\pm 0.1\times10^{-3}$) gm Selenium and 4.489 ($\pm 0.1\times10^{-3}$) gm Tellurium are mixed in a tube of Pyrex and it was put it in the vacuum system at 10^{-2} m bar pressure, then the tube was put it in the oven and heated to 550 ^{o}C, (this degree was higher than the melting point of Tellurium which was 452 ^{o}C). The tube was leaved in the oven for eight hour with stirring form time to time, then the alloy Quenched(cool suddenly) in cold distilled water then left it to dry. These films were prepared at different substrate temperature between room temperature (RT), 50 ^{o}C, 100 ^{o}C and 150 ^{o}C that by using heater before the deposition process.

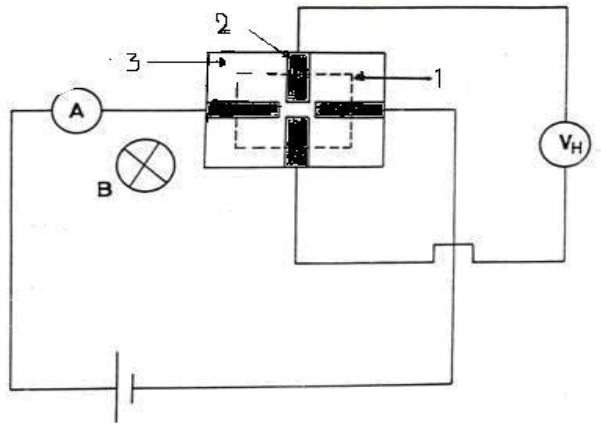


Fig. (1):The circuit diagram of Hall measurement. (A): Ammeter, (V_H): Voltmeter, (B): Magnetic Field

1- doted square is the films.

2- dashed lines represent the mask.

3- The Aluminum substrate.

The electrodes, which were used for Hall measurements and for electrical measurements made from Aluminum films by using the vacuum coating system type "Edwards E 306A", with the help of special masks, as shown in Fig.(1), the evaporation condition was don in high vacuum condition at pressure and it was equal 4×10^{-6} m bar.

Some of the prepared films of $Se_{0.3}Te_{0.7}$ were annealed at 200^{o}C degree to study the properties and structure of the annealing film.
Part of the $Se_{0.3}Te_{0.7}$ alloy was smash to get the powder of the alloy in order to study the structure of the alloy by using X-ray diffraction method.

The thickness of the prepared films was measure by using two methods; the weight method and optical interference method. Weight method gives an approximate value for the thickness of the thin films with an error 30 % but it is necessary to calculate the quantity of the evaporate material to get the suitable thickness of the film.

Result and Discussions

1. X-ray diffraction test

The powder of SeTe alloy, which was prepared as thin films, was tested by X-ray diffractions. By coincide the results with publications table for this alloy; it was found to be $Se_{0.3}Te_7$ compound. Table (1) shows the information that taken from X-ray diffraction file about the prepared film and the information that taken from the scientific literature about the same compound [9, 17, 18]. The prepared alloy coincide the standard specifications.

Table (1)
The information of $Se_{0.3}Te_{0.7}$ alloy that was calculated from the X-Ray diffraction and from the reported papers [9, 15, 16].

hkl	d (Calculate)nm	d (Stander)nm
100	0.3896	0.3849
101	0.3252	0.3194
102	0.2313	0.2297
110	0.2262	0.2222
111	0.2099	0.2087
201	0.1848	0.1838

The disappearance of peaks (201), (111), (102) in X-ray diffraction pattern, as shown in Fig.(2), explain the structure of the prepared

film at room temperature, part of it was amorphous and another part was polycrystalline.

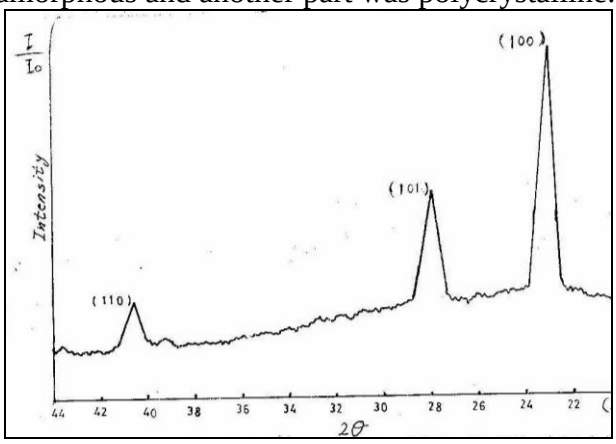


Fig. (2): X-ray diffraction pattern of $Se_{0.3}Te_{0.7}$ thin film prepared at room temperature.

The deposit films at different substrate temperature have great effect on $Se_{.3}Te_{.7}$ structure and that could be observed from the X-ray diffraction pattern, the crystallization state of the films decrease when the substrate temperature.

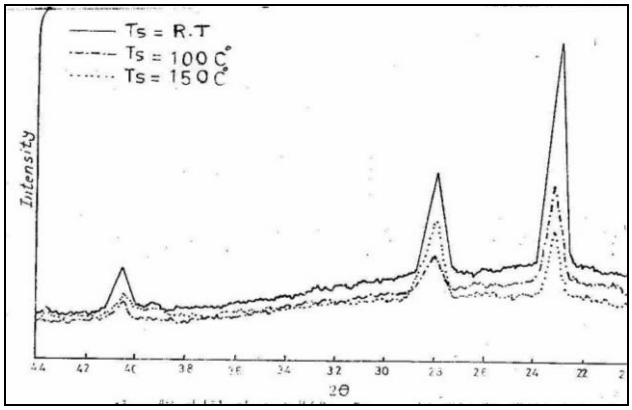


Fig. (3): X-ray diffraction pattern of $Se_{0.3}Te_{0.7}$ thin film prepared at different substrate temperature.

Fig.(3) shows the drop of the Brack peaks at substrate temperature 100°C, 150 °C, that mean the temperature can help in arranging the bonds between the atoms and this temperature gives energy to Se atom in order to separate the connection between Se atom with Te, (weakness of Se-Te bonds) and then Se will union with Se atom, that will generate island in the film and that will decreasing the crystallization state of the film.

The annealing has affect on the crystallization structure of the prepared film. X-ray diffraction pattern of the annealed films was studied; the results shows increasing in the crystallization state at 100 °C because of the union between Se atom with Se atom, then the crystallization go down at 200 °C that mean Se atoms arranged the bonds to be more connected with the alloy.

2. Calculation the concentration of charges carriers

Hall measurement was used in order to know the concentration and the type of charge carriers of $Se_{0.3}Te_{0.7}$ films, the results of Hall effect measurements at room temperature are plotted in Fig.(4). The concentration of charge carriers was calculated by using equation 5; (the value of the used magnetic field was 0.194 Tesla), the charge carries of the prepared films at different substrate temperature (R.T, 50, 100, 150) °C have positive value; that means all the prepared films were p-type.

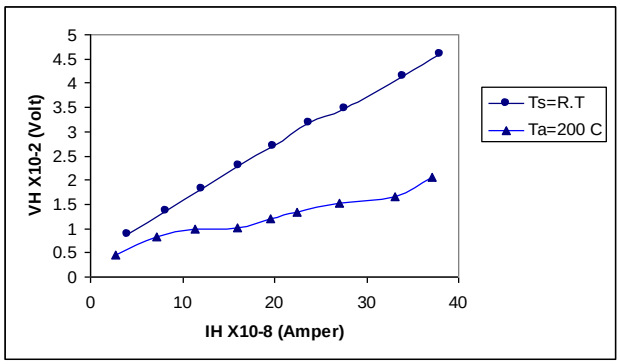


Fig.(4) : Hall Effect measurements at room temperature and at annealing temperature 200 °C.

The results of the Hall effect measurements was listed in Table (2), there was decreasing in concentration of charges carriers when increasing the substrate temperature. In addition, the concentration of charges carriers of the annealed film at 200 °C was decreases.

(c); Ts=100 °C.

Table (2): The optical energy gap of $Se_{.3}Te_{.7}$ films p

Figs. (5-a, b, c, d): The optical energy gap of $Se_{.3}Te_{.7}$ films p

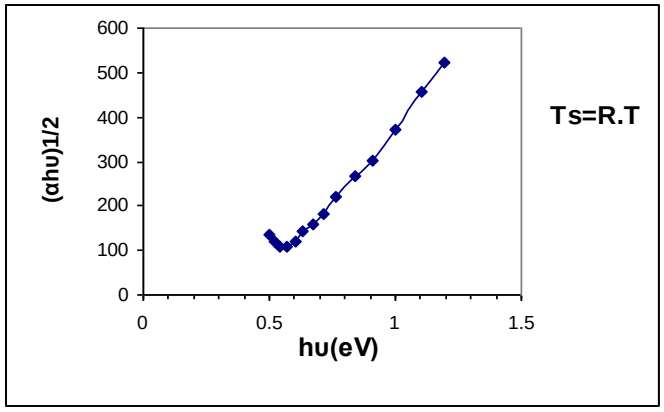
The changes of Hall coefficient values and the concentration of charges carriers at different substrate temperature.

$Se_{0.3}Te_{0.7}$			T(Anneal) 200 °C	
Ts °C	RH $cm^3.C^{-1}$	N cm^{-3}	RH	N cm^{-3}
25	0.083	7.48×10^{19}	0.31	2.0×10^{19}
50	3.01	2.05×10^{19}	3.48	1.79×10^{19}
100	3.78	1.65×10^{18}	3.98	1.56×10^{18}
150	3.86	1.61×10^{18}	3.18	1.01×10^{18}

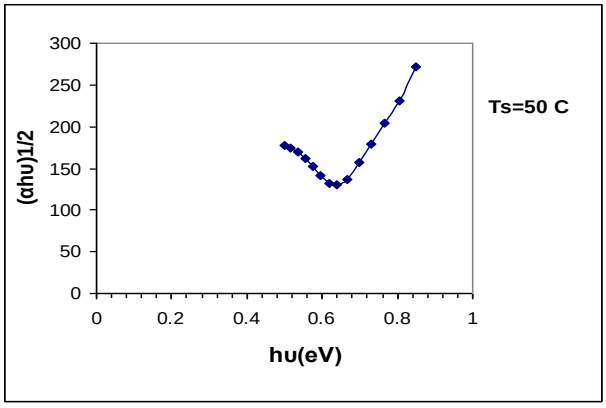
3. Calculate the values of the energy gap at different substrate temperature

The energy gap can be calculated from the diagram of the relation between hν and $(\alpha h\nu)^{1/2}$ among the extension of the linear part at $\alpha h\nu = 0$, (see equation 1).

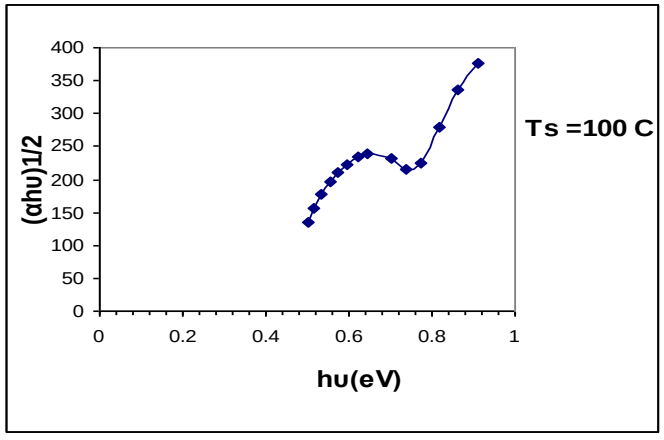
The results assured that electrical transitions in $Se_{.3}Te_{.7}$ films were indirect transitions, as shown in Figs. (5-a, b, c, d), the energy gap of the annealed film at 200°C was calculated too, as shown in Fig.(6).

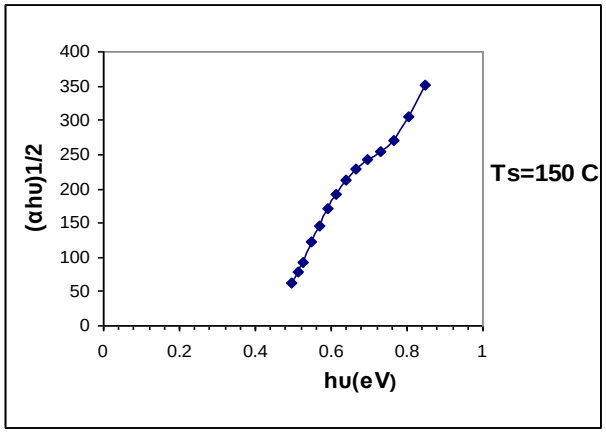


(a); Ts= room temperature.



(b);Ts=50 °C.





(d); Ts=150 °C.

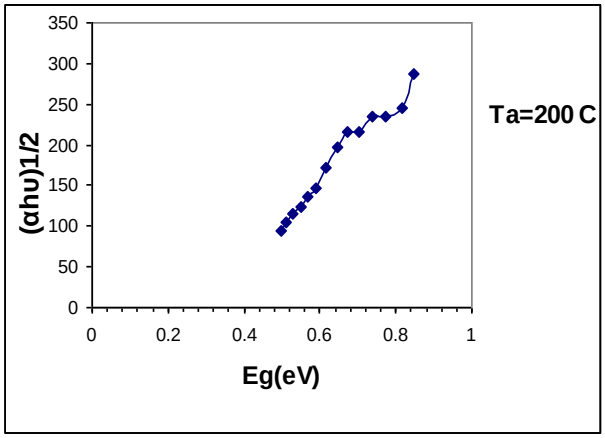


Fig.(6): The optical energy gap of the annealed $Se_{.3}Te_{.7}$ films Ts=R.T, Ta=200 °C.

The optical energy gap of prepared $Se_{.3}Te_{.7}$ film at room temperature was 0.48 eV which is less than the energy gap of Selenium (1.86eV) and the energy gap of Tellurium (0.33)eV, so that the addition of Selenium to Tellurium expand the optical energy gap.

The optical energy gap values of $Se_{.3}Te_{.7}$ film were calculated at different substrate temperatures; (R.T, 50, 100, 150) °C, as listed in Table (3).

Table (3)
The values of the optical energy gap at different substrate temperature for the annealed and unannealed $Se_{.3}Te_{.7}$ film.

$Se_{0.3}Te_{0.7}$		
T(substrate) °C	Eg (eV)	Eg (eV) (annealing) Ta=200 °C
R.T=25	0.48	0.62
50	0.50	0.64
100	0.54	0.66
150	0.56	0.68

The substrate temperature has affected on the value of the energy gap, the connection of Se atom with Te atom will separate at increasing the temperature, then Se atom will union with Se atom, so the crystallization state decrease, (as mentioned before), for that reason; the value of the energy gaps will increases.

The results of the annealed film at 200°C for 60 minute shows the increasing in optical energy gap about (0.14)eV, that mean the annealing process increase the crystallized grain size and decrease the defects of the structure of the films.

4. Measurements of the refractive index

The refractive indexes (n) of the prepared $Se_{.3}Te_{.7}$ films are plotted as a function of the wavelength at wavelength 2100 nm at different substrate temperature, as shown in Fig.(7).

The refractive index of the film at room temperature was 4.2 at wavelength 2100 nm; this wavelength is approximately in the middle of the used spectrum region (1500-2500) nm and the result was near with results of the other researchers [8].

In addition, the results show that the substrate temperature has an effect in decreasing the value of the refractive index, the decreasing continuous with the increasing of the substrate temperature, as listed in Table (4).

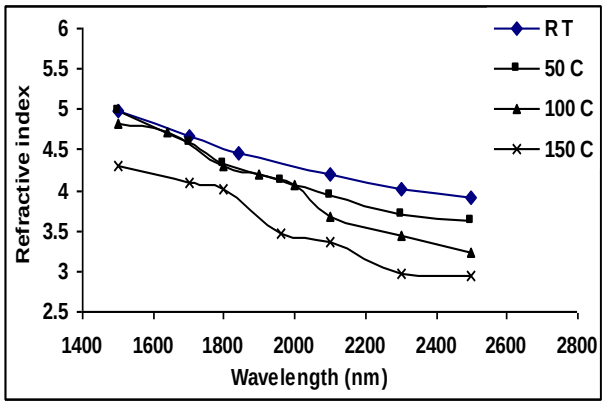


Fig. (7) : The values of refractive index of $Se_{0.3}Te_{0.7}$ films at 2100nm wavelength at different substrate temperature.

5. Measurements of the dielectric constant

Dielectric constant defines as the response of the material toward the incident electromagnetic field. Dielectric constant value for $Se_{0.3}Te_{0.7}$ film

was change at different substrate temperature, (R.T, 50, 100, 150) ^{o}C.

The real and the imaginary dielectric constant were calculated, and listed in table 4. The value of the real part of dielectric constant ϵ_1 was depending on the value of the refractive index, it was decrease at the increasing of the substrate temperature.

Table (4)
The values of the refractive index and dielectric constant for $Se_{.3}Te_{.7}$ film at 2100nm wavelength at different substrate temperature.

$Se_{0.3}Te_{0.7}$ At wavelength 2100 nm				
Ts ^{o}C	B×10^5 (eV.cm) $^{-1}$	n	ϵ_1	ϵ_2×10^2
RT	7.97	4.20	17.69	11.44
50	9.07	3.94	15.52	9.06
100	16.45	3.66	13.39	9.53
150	23.15	3.35	11.22	7.16

Conclusions

The annealing of $Se_{0.3}Te_{0.7}$ film at 200 ^{o}C has an effect on the crystallization structure of the film. The optical energy gap of the prepared films has different values at different substrate temperature, the value of the refractive index decrease at the increases of the substrate temperature.

References

[1] R. Chiba and N.Funakoshi, (1988), "Thin Solid Films", Vol. 157. pp. 307-313.
[2] D. E Carlson, (1980), "Polycrystalline and amorphous thin films and devices, "Ed. L. L. Kazmeraski, Academic press.
[3] F.M. Mehra" A.Ganjeo and P.C Mathur, (1994). "J.Appl. phys" Vol. 11, pp. 7334-7339.
[4] M. H. Brodsky, (1979), "Topics in applid physics amorphous semiconductor", Vol. 36.
[5] A. H. Abouelela, M. K. Elmously and K. S. Abdu, (1980), "J. Matter. Science" Vol. 15, pp. 871-874.
[6] R. M. Mehra, Radhey Shyom and P.C. Mathur, (1979), "Phys. Rev. B" Vol. 19, pp. 6525-6531.
[7] H. Watanabe and K. C. Kao, (1979), "Jap. J. Appl. Phys.", Vol. 18, pp. 1949-1850.
[8] N.D. Mott and E. A. Davis, (1971),"Electronic processes in Nano Crystalline Materials Oxford University prese.
[9] H. P. D. Lanyon, (1964), "J. Appl. Phys ", Vol. 35, pp. 1516-1523.
[10] A. L. Dawar, J. C. Joshi and L. Noroin, (1981), "Thin Solid Film ", Vol. 76, pp. 113-117.
[11] H. Adachi and K. C. KAO,(1980), "J. Appl. Phys. ", Vol. 51, pp. 6226-6330.
[12] S. Lindroos and G. Rusu, (2005), "J. Optoelectronic. Adv. Materials", V. 7, No. 2, P. 817.
[13] J. Singh, (2006), "Optical Properties of condensed Matter and applications", John wiley & Sons.
[14] D. Emin, (1980), "Polycrystalline and amorphous thin films and devices", ed. L. L. Kazmaraski, Academic press.
[15] I. S. Athwa, Jaswinde and R. K. Bedi, (1989), "Thin Solid Film", Vol. 162, pp. 1-6.
[16] Alexis De Vos and J. Aertes, (1988), "Thin Solid film, Vol. 46, pp. 223-228.
[17] V. Damodara Das, J. K. Mukuerjec and D. N. Bose, (1987), "J. Mater. Sci" Vol. 22, pp. 23772381.
[18] V. Damodare Das and P. J. Lakshmi, (1988), "J. Mater Sci", Vol. 23, pp. 3869-3875.

الخلاصة

في هذا البحث تم تحضير سبيكة $Se_{0.3}Te_{0.7}$ من خلط أوزان دقيقة وبنسب معينة من مادتي السلينيوم Se والتريليوم Te عاليي النقاوة باستخدام تقنية التبخير الفراغي, تم تحضير الأغشية عند درجات حرارة أساس مختلفة

(25, 50, 100, 150) ^{o}C وتم تلدين بعض من الأغشية المحضرة لدرجة حرارة 200 ^{o}C.

تم اخذ عينة من مسحوق السبيكة المحضرة وتم فحصها بطريقة حيود الأشعة السينية وتبن من تحليل النتائج إن جميع الأغشية هي نوع متعدد التبلور polycrystalline , ومن نتائج معامل هول Hall Factor تبين بأنها نوع p (p-Type), تم حساب تركيز حوامل الشحنات وتبين أنها تقل عند الغشاء الملدن.

تم دراسة الخواص البصرية لسبيكة $Se_{0.3}Te_{0.7}$ المحضرة على شكل أغشية رقيقة, و تم حساب قيم فجوة الطاقة البصرية وكانت قيمتها تساوي 0.48 eV عند درجة حرارة الغرفة, وقد تبين ان هذه القيمة تزداد عند زيادة درجة حرارة الأساس أثناء التحضير, تم أيضا قياس قيمة فجوة الطاقة البصرية للغشاء الملدن عند درجة 200 C^{o} وكانت تساوي 0.62 eV. تم أيضا حساب معامل الانكسار أغشية السبيكة المحضرة بدرجة حرارة الغرفة كدالة للطول ألموجي 2100 nm وكانت قيمته تساوي 4.2.