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Annealing Effect on Optical properties of ($As_{0.5}Se_{0.5}$ doped with 1% Te) thin films

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Abstract:

this work, the study of optical properties of ($As_{0.5}Se_{0.5}$ doped with 1% Te) thin films which prepared by thermal vacuum evaporation on glass bases at (R.T) with (100±20) nm thickness deposition rate (1.6nm/s) and study effect of annealing at temperatures (Ta) (348,398,448) K for time (30min) on these properties. The X-ray diffraction technique showed that all prepared films are amorphous in structure at room temperature and annealing films at (348, 398, 448) K. The transmittance spectra of the prepared films fall within a wavelength range (500-1100) nm, and increasing the annealing temperature leads to a decreased in transmission, increased absorption coefficient, and shift of the absorption edge towards low photon energies. The optical measurements showed that the prepared films had an allowed indirect optical energy gap and were found to decrease with the increase of (Ta) within the range (R.T, 348,398,448) K. As indicated by the tails of the localized states, it was observed that they increased by increasing (Ta).

Key words: chalcogenide glass, localized states, absorption coefficient, annealing.

تأثير التلدين على الخصائص البصرية لأغشية (As0.5Se0.5المشوبة ب 1% Te)

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الخلاصة:

تم في هذا البحث دراسة الخصائص البصرية لأغشية As0.5Se0.5) المشوبة بالتيليريوم بنسبة 1%) الرقيقة المحضرة بطريقة التبخير الحراري في الفراغ على قواعد زجاجية بدرجة حرارة الغرفة وبسمك (100±20)nm وبمعدل ترسيب (nm/s1.6)، ودراسة تأثير التلدين عند درجات حرارة (348,398,448)K) (Ta ولمدة (min30) على الخصائص قيد البحث. تبيّن من خلال نتائج حيود الاشعة السينية (XRD) ان جميع الاغشية كانت عشوائية التركيب عند درجة حرارة الغرفة (R.T) والاغشية الملدنة ضمن المدى (348,398,448)K. وان طيف النفاذية للأغشية المحضرة يقع ضمن مدى طول موجي (500-1100)nm، وان زيادة درجة حرارة التلدين تؤدي الى نقصان النفاذية (زيادة في الامتصاصية) وزيادة معامل الامتصاص وازاحة حافة الامتصاص نحو الطاقات الفوتونية الواطئة. واظهرت القياسات البصرية ان للأغشية المحضرة فجوة طاقة بصرية غير مباشرة مسموحة ووجد انها تتناقص مع زيادة (Ta) ضمن المدى R.T,348,398,448)K) كما حُسب عرض الذيول للحالات الموضعية ولوحظ انها تتزايد بزيادة (Ta)

الكلمات الرئيسية: زجاجيات الجالكوجينات، المستويات الموضعية، معامل الامتصاص، التلدين

Introduction:

Thin-film occupies a prominent place in theoretical and applied research of solid state physics, as a result of continuing research on the physical properties of the material at the last decades of the last century physics branch appeared thin films of materials science, which means study systems of different elements and compounds easily and the advantage of the lack of preparation costs and the possibility of preparation modalities and the dimensions are very familiar. As it can be described as a single layer or multiple layers of atoms of a particular substance does not exceed a thickness Macron one, we know the physical and chemical properties of materials that cannot be studied in some cases, which is in its volumetric [1]. The glasses (As-Se-Te) is a great significance in terms represent a new classification for semiconductor and its thin films used in many technological and scientific applications, where used in optical memory devices, photographic printing to the advantage of its high sensitivity when exposed to a wavelength identical to the energy gap. (Popescu) [2] found that most chalcogenide glasses films that doped with (Te) uses in medical diagnosis and in pollution monitoring. The common feature of these glasses is the presence of localized states in the energy gap because of the absence of long-range order as well as various inherent defects. Recently, the investigation of electron transport in disordered system has gradually been developed and the investigation of gap states is of particular interest because of their effect on the properties of semiconductors [3]. Process of exposing the film to a certain temperature in a specific period of time called the annealing has been carried out either in vacuum or in presence of a particular gas or in air. The annealing granted atoms kinetic energy that necessary to rearrange itself in the crystalline lattice that is lead to organization of the crystal structure of the material and reduces the defects. (Hsiuang and Wang) [4] found the effect of thermal treatment on amorphous semiconductors will be in two phases: the first includes the reduction in the disordered of atoms (at low temperature), the second phase include reducing the dangling bonds (at high temperature). Studying the effect of annealing temperature on the optical properties provides a better understanding mechanism of disorder and defect formation in the chalcogenide films.

Experimental

The glassy alloys of ($As_{0.5}Se_{0.5}$ doped with Te at 1%) were prepared by applying melt quenching technique. The exact proportions of high purity (99.999%) arsenic (As), Selenium (Se) and tellurium (Te) elements, in according with their atomic percentages, and put these elements in quartz tube sealed at (10^{-2}torr). The tube was heated to (823k) for (4-5 hours) and shaken it several times during the course of heating to attain uniformity. The molten samples were then rapidly quenched in cold water. The films of ($As_{0.5}Se_{0.5}$ doped with 1% Te) of thickness (100±20) nm were prepared by vacuum evaporation technique using molybdenum boat according to low [5]: ($m = 2\pi\rho_0 r^2 t$) where m: weight of alloy, r: the distance from boat to a substrate, t: the thickness of film. ρ_0: the density of alloy ($\rho_0 = \frac{m_T}{V_T}$) where m_T: the alloy mass, V_T: the alloy volume. The films of ($As_{0.5}Se_{0.5}$ doped with 1% Te) were annealed at (T_a) (348,398,448) K by using oven type of (Griffin Incubator) which reaches the great degree of temperature at (473K).

Results and Discussion

Transmittance(T_o)and Absorbance (A_o):

Non-crystalline was tested for ($As_{0.5}Se_{0.5}$ doped with 1% Te) film by x-ray diffraction

even after annealing films at ($T_a = 348{,}398{,}448$) K. The well-defined peaks characteristic of crystalline materials was absent. It can be found many optical constants through study the transmittance and the absorbance of wide ranges of wavelengths. Fig. (1) show x-ray diffraction scheme of the films of ($As_{0.5}Se_{0.5}$ doped with 1% Te) were annealed at (T_a) (348,398,448) K.

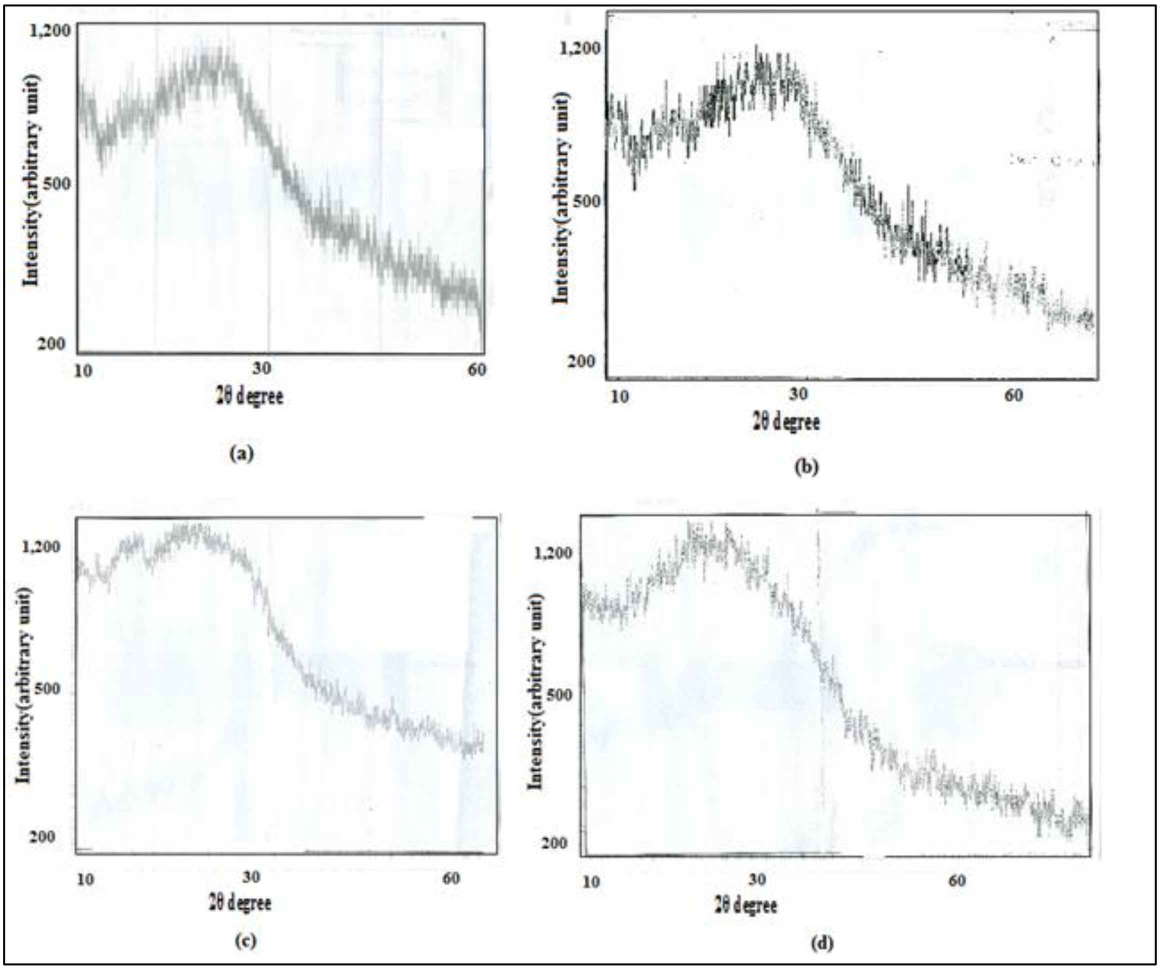

Fig-1: XRD pattern of the films of ($As_{0.5}Se_{0.5}$ doped with 1% Te): (a) at R. T=303K. (b) at $T_a = 348K$. (c)at $T_a = 398K$. (d) at $T_a = 448K$.

Figure -2 shows transmittance spectra as a function of wavelength of (As0.5Se0.5 doped with 1% Te) film deposited at room temperature and annealed at ($T_a =$ 348,398,448)K at wavelength range (500-1100) nm, where we note that increase the transmittance of all prepared films with increasing wavelength, while the transmittance curve decrease with increase the annealing temperature because of the large size crystals of film material. The films transmittance within the region near infrared spectrum, this is consistent with the results of previous works [6-10].

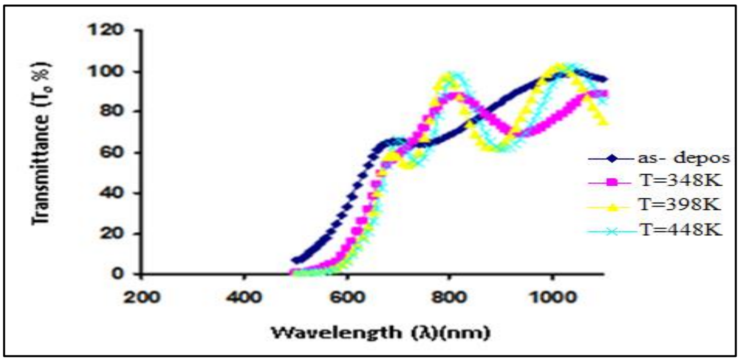

Fig-2: transmittance (T_0) as a function of wavelength (λ) for prepared and annealed of ($As_{0.5}Se_{0.5}$ doped with 1% Te) films.

Fig. (3) shows the absorbance spectra as a function of wavelength for a prepared and annealed films of ($As_{0.5}Se_{0.5}$ doped with 1% Te) with different annealing temperature ($T_a = 348,398,448$) K, it has been observed that all prepared films characterized by high absorb at short wavelengths, this is behaving just opposite what we have observed in the transmittance curves, and the absorption spectrum of this films is located within the visible region.

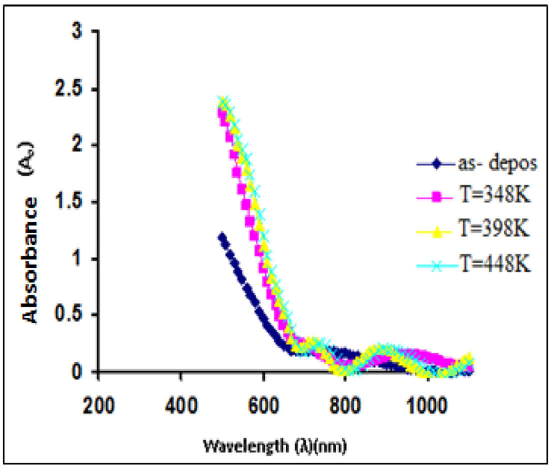

Fig-3: Absorbance (A0) as a function of wavelength (λ) for prepared and annealed of ($As_{0.5}Se_{0.5}$ doped with 1% Te) films.

Absorption Coefficient

It has been using the absorbance data (A_0) to calculate the absorption coefficient (α) as in equation (1)

$$\alpha = 2.303\frac{Ao}{t} \quad \dots\dots\dots\dots\dots\dots\dots\dots.(1)$$

Where t: is film thickness.

Figure (4) shows the change in the absorption coefficient (α) with the photon energy (hυ) for a prepared and annealed films of ($As_{0.5}Se_{0.5}$ doped with 1% Te) with different annealing temperature ($\boldsymbol{T_a} = \mathbf{348, 398, 448}$) K, the absorption coefficient increases with the photon energy of all films, we also find the appearance of convex clearly at low photonic energies, The reason for this convexity is the presence of absorption peaks located in the low-energy side of the absorption edge of some materials, this means the absorption of photons with energies less than the energy of the optical gap by a certain amount [11]. The presence of local energy levels between the valence and conduction bands results in electron transitions between the valence band and these local levels or between these local levels and conduction band the absorption of this transition is weak and involves a small amount of energy compared to the absorption of electronic transitions between energy bands (conduction and valence) because the density of states for these levels is less than the density of states for conduction and valence bands, and this phenomenon often occurs in random materials. Also, can observe from fig. (4) that annealing process causes creep absorption edge towards low photon energies and increasing the absorption coefficient for annealing films, a sign of a decrease in the energy gap after the process of annealing, this is due to the increased width of the edge of the bands (valence and conduction) within the gap due to contamination during the process of annealing [12, 13].

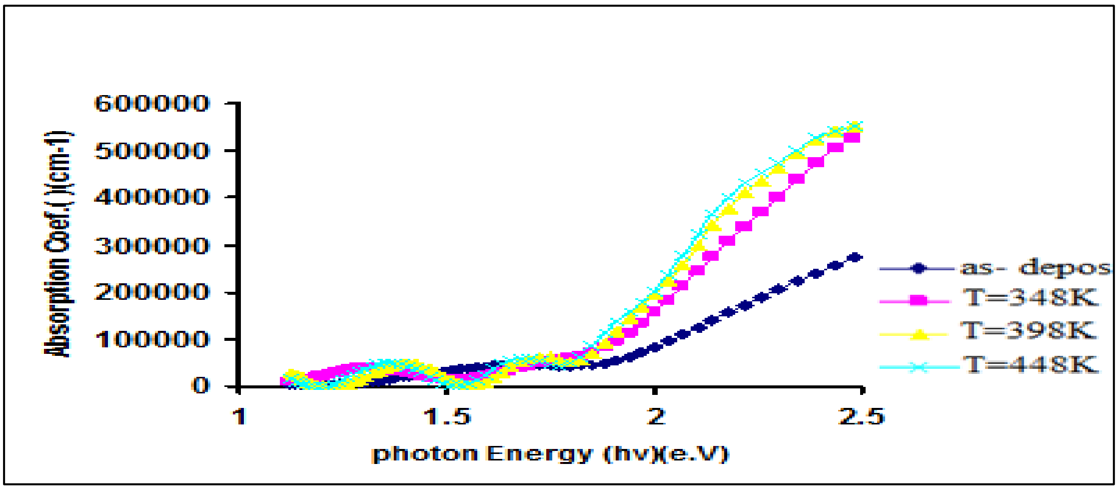

Fig-4: Absorption coefficient (α) as a function of photon energy (hυ) for prepared and annealed films of (As0.5Se0.5 doped with 1% Te).

Optical Energy Gap (E_g^{opt})

The most advanced research [7,9,14] has shown that the electronic transitions of the chalcogenide system of (As-Se-Te) films are indirect allowed.

The optical energy gap (E_g^{opt}) was calculated for the indirect allowed transition from equation (2):

$$(\alpha h\upsilon)^{\frac{1}{2}} = A^{\frac{1}{2}}(h\upsilon - E_g^{opt}) \quad \ldots\ldots\ldots (2)$$

Fig.(5) represent the change $(\alpha h\upsilon)^{\frac{1}{2}}$ with photon energy ($h\upsilon$) for the prepared and annealed films of ($As_{0.5}Se_{0.5}$ doped with 1% Te) with different annealing temperature ($T_a = 348,398,448$) K at (30 min), and from Table (1) it can be observed that the value of energy optical gap (E_g^{opt}) for indirect allowed transition decrease with increasing annealing temperature of the prepared thin films, this is consistent with (Dongol)[12], (Nyakotyo, et al.) [15], (pathak et al.)[16]. It can be explained by the fact that annealing process increased local levels near the valence and conduction bands and thus reduced the optical energy gap.

The relationship between $(\alpha h\nu)^{1/2}$ as a function of the photon energy ($h\nu$), where $A = (slope)^2(cm^{-1}.eV^{-1})$, and we found that the value of the constant (A) decreases by increasing the temperature of the annealing, ie, the films is highly randomized by increasing the (T_a) because constant (A) is a measure of the randomness of the film [17]. This confirms our results, as shown in Table-1.

Table -1: The values of E_g^{opt}, and constant (A) of ($As_{0.5}Se_{0.5}$ doped with 1% Te) thin films at different annealing temperatures

$As_{0.5}Se_{0.5}Te_{0.01}$ Thin Film	at R. T=303K	T_a 348K	T_a 398K	T_a 448K
$E_g^{opt}(eV)$	1.72	1.63	1.59	1.55
A ($cm^{-1}.eV^{-1}$)	$2.25*10^6$	$1.96*10^6$	$1.77*10^6$	$1.56*10^6$

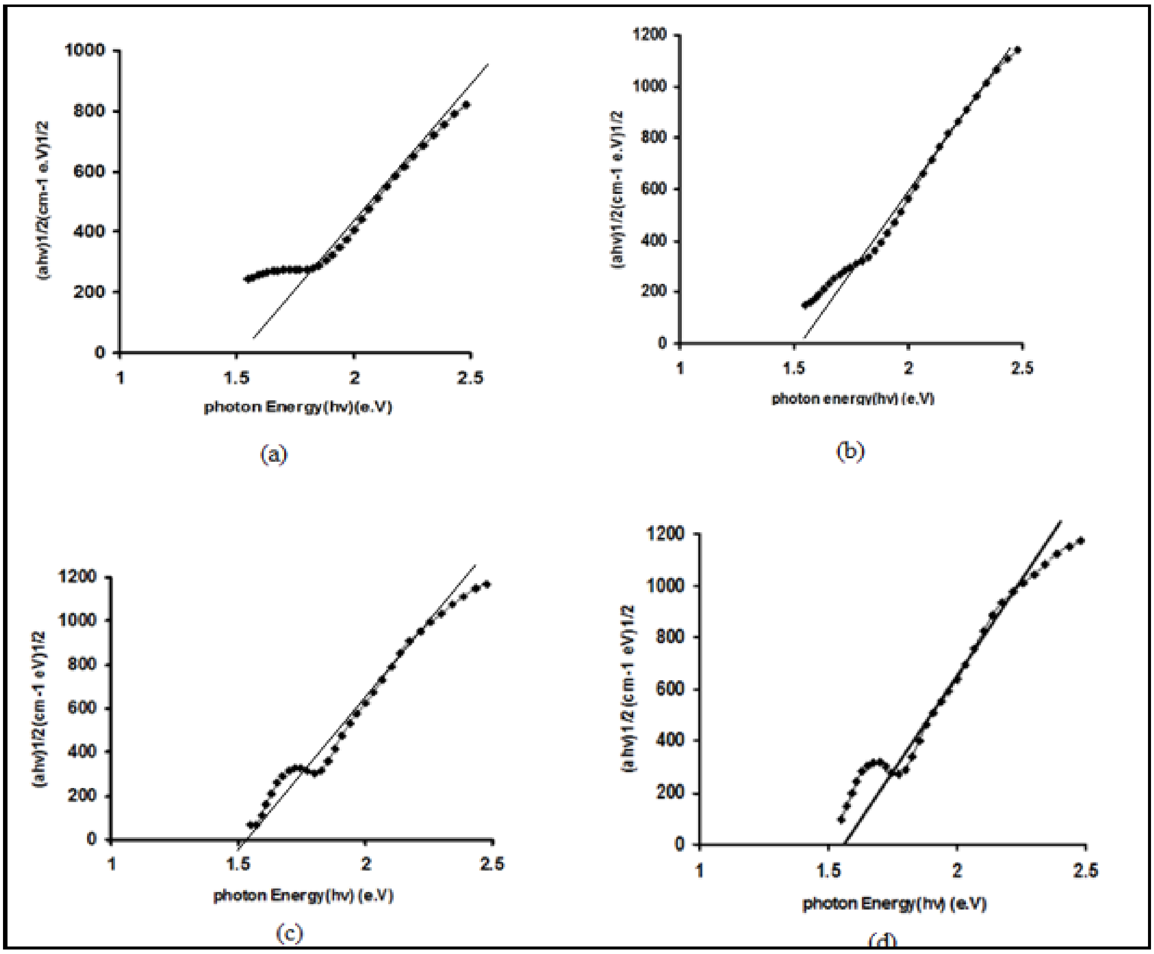

Fig -5: $(\alpha h\upsilon)^{\frac{1}{2}}$ versus photon energy $(h\upsilon)$ of ($As_{0.5}Se_{0.5}$ doped with 1% Te) thin films (a) at R. T=303K. (b) at $T_a = 348K$. (c) at $T_a = 398K$. (d) at $T_a = 448K$.

Calculated Tails Width for Localized states (ΔEe)

To calculate the tails width of the localized states (ΔE_e) within the energy gap called the Urbach tails, the equation (3) was used

$$ln\alpha = ln\alpha_o + h\upsilon/\Delta E_e \qquad \dots(3)$$

Therefore, when plotting the relationship between $(ln\alpha)$ and photon energy $(h\upsilon)$ for ($As_{0.5}Se_{0.5}$ doped with 1% Te) at room temperature and annealing at (348,398,448) K for 30 min, as fig. (6) and inverted the inclination of the linear part of the graphic curve was found in the Urbach tails (ΔE_e). Table (2) shows the results, where the value of (ΔE_e) for all the films is within the range of tails width for amorphous semiconductors (0.05-0.8) eV [18], also find (ΔE_e) of the prepared films increases by increasing the temperature of annealing. The reason for this increase is the increase in local levels at the edges of the bands (valence and conduction) as well as the defect levels in the gap that are attributed to the Dangling Bonds and Wrong-Bonds this means the increase of random films by increasing the temperature of annealing and then decreasing the optical energy gap.

Table -2: Urbach tails (ΔE_e) values of ($As_{0.5}Se_{0.5}$ doped with 1% Te) thin films at different annealing temperatures.

$As_{0.5}Se_{0.5}Te_{0.01}$ Thin Film	at R.T=303K	T_a 348K	T_a 398K	T_a 448K
ΔE_e(eV)	0.233	0.250	0.268	0.288

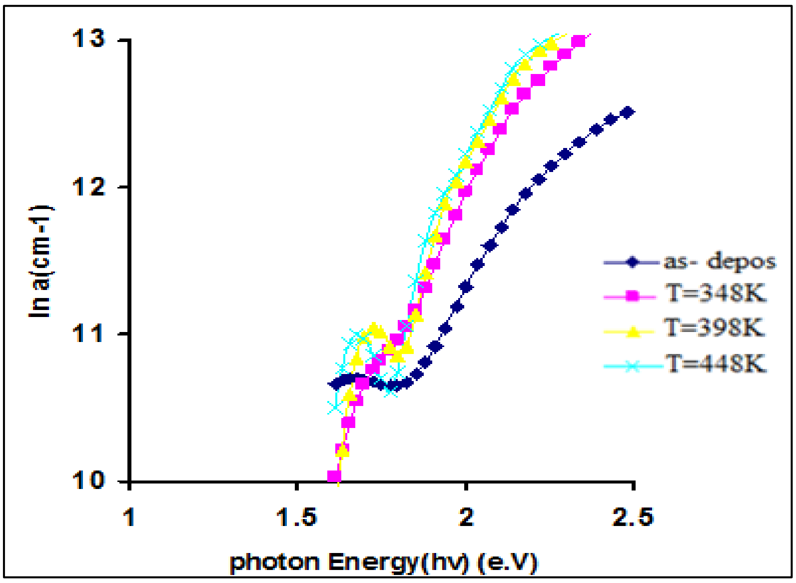

Fig-6: ($ln\alpha$) versus photon energy ($h\nu$) for a prepared and annealed of ($As_{0.5}Se_{0.5}$ doped with 1% Te) films.

Conclusions

Amorphous thin films of ($As_{0.5}Se_{0.5}$ doped with 1% Te) were obtained by thermal evaporation technique on glass substrates. From the study of optical properties of the prepared films show that the transmittance of the films lies within the near infrared region of the spectrum. Absorption decreases with the increase of wavelength and falls within the visible area of the spectrum. Increasing the temperature of the annealing leads to decreased transmission and increased absorption coefficient and shift the absorption edge towards low photonic energies. By increasing the temperature of annealing leads to a decrease in the indirect optical energy gap and increased band tails width. The ($As_{0.5}Se_{0.5}$ doped with 1% Te) films can be used to produce solar cells for its height transmittance in infrared region of spectrum.

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