Study the effects of annealing temperature on some optical properties of Se:2%As thin films

*G. H. Mohammed

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Abstract:

The optical gap (E_{opt}) and tailing(ΔE) for Se:2%As thin films prepared by vacuum evaporation as a function of annealing temperature are studied in the photon energy range (1.0 to 5.4) eV. Thin film of Se:2%As was found to be indirect gap with energy gap of (1.978 , 2.082 , 2.120 , 2.230) eV at annealing temperature (295 , 370 , 445 , 520)K respectively.

The E_{opt} and ΔE of Se:2%As films as a function of annealing temperature showed an increase in E_{opt} and a decrease in ΔE with the temperature. This behavior may be related to structural defects and dangling bands. The absorption coefficient for Se:2%As films exhibits exponential dependence on photon energy obeying Urbach's rule in the absorption edge.

Introduction:

It will know that the structure and properties of amorphous semiconductors are sensitive to the method of preparation [1]. For example, evaporated films of germanium and arsenic chalcogenides have X-ray-diffraction and optical absorption properties that are significantly different from the corresponding bulk glasses [2-3]. However, annealing temperature reduces this difference, and the properties of the resulting annealed films are indistinguishable from those of bulk glasses.

The trigonal Se is made of Se chains, while monoclinic Se is composed of Se_8 rings with different stacking of the rings. A-Se has often been taken as being a mixture of Se chain and Se_8 rings [4].Selenium is a typical chalcogenide glassy semiconductor and is contain two kinds of molecule, polymeric chains and nonnumeric rings and inherent defect states called valence-alternation pairs (VAP). The creation of VAPs is described by reaction[5]:

$2Se_2^{o}=Se_1^{-}+Se_3^{+}$

Where the subscripts denote the covalent coordination and the superscripts- the charge states

Optical properties of V-VI compounds have been studied in various publication [6-9]. The optical band gap and the localized states width are found to depend on the composition. Still the properties of the prepared materials are highly dependent on the preparation condition, leading to difference in the values of the parameter connected with electrical properties, optical properties, glass transition temperature, crystallization ... etc.

The optical absorption coefficient for many amorphous and glassy materials is found to obey the relation[10-11] :

$(\alpha h\upsilon)=\beta\,(h\upsilon - Eopt)^{r}$ ----------------(1)

where β is a constant, r is a number between 1 and 3 and Eopt is the optical energy gap.

*Department of Physics ,College of Science, University of Baghdad , Jadirya-Baghdad-IRAQ.: e- mail: ghusson_hameed@ yahoo.com

The relation was first derived by Tauce and Colleagues [12] who assumed that the electron density of states at band edges in regions of localized states is a parabolic function of energy. Davis and Mott[13] obtained the same relation. The width of the tails of localized states at the band edges can be estimated using the Urbach relation [10]:

$(\alpha h\upsilon) = \alpha_0 \exp(h\upsilon/\Delta E)$ ---------------(2)

where α_0 is a constant and ΔE is a measure of the extent of the band tailing in the band gap of the material and determined from the reciprocal of the slope of Lnα against photon energy.

This report will give results of a systematic study of the optical properties of Se:2%As amorphous thin films at different annealing temperature (295,370,445,520)K.

Experimental:

The materials are (99.999% in purity), were prepared at room temperature by thermal co-evaporation technique from two molybdenum boats in a vacuum at a pressure of about ($5x10^{-6}$)Torr using Edwards coating unit E 306. The films thickness was accurately determined using Tolonsky methods.

The glassy nature of the samples was investigated using X-Ray diffraction. Spectral characteristics were measured using UV-visible recording spectrophotometer (UV-160 Schematize). The measurements were carried out in wavelengths in the range (200-1100) nm. The samples were thermally annealed at different temperature.

The absorption coefficient (α) calculated from the relation:

$\alpha = 2\cdot303$ (A/t) -----------------------(3)

where A was the absorbance and t was the thickness of the films.

Results and discussions:

X-ray analysis at room temperature showed the absence of any peak, which indicated that the films were amorphous.

The absorption coefficient:

Fig.(1) shows the plots of absorption coefficient (α) versus photon energy ($h\upsilon$) at different annealing temperature. As evident from this figure that the absorption coefficient (α) varies exponentially with ($h\upsilon$) in the measured of absorption edge. It can be observed that there is regular shift of the absorption edge to higher photon energy, when evaporated films are annealed. The shift in the absorption edge due to the heat treatment is explained by a change in the defect structure of the films [13]. The absorption edge at room temperature is in a good agreement with the result on Se:2%As glass reported by Kolomiets et.al.[14].

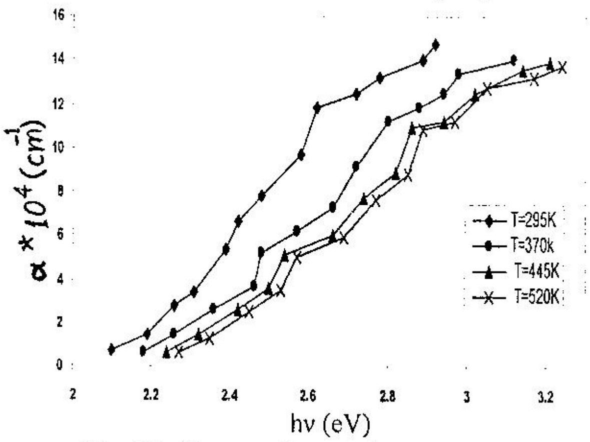

Fig.(1) Shows the variation of α with photon energy for Se:2%As films at different annealing temperature.

The Energy Gap:

As explained by Taus [1], there are three different regions in the optical absorption curve for an amorphous semiconductor corresponding to three different range of absorption coefficients. In the first region corresponds to an absorption $\alpha < 1cm^{-1}$, the second region corresponds to an absorption in the range $1< \alpha >10^4$ cm^{-1} . A high value for absorption coefficient marks the third region [1].

The value of the optical gap E_{opt} in the amorphous materials is obtained by plotting $(\alpha h\upsilon)^{1/r}$ and $h\upsilon$ (r=1/2,3/2,2,3) followed by extrapolating the linear region of the plot of $(\alpha h\upsilon)^{1/r}=0$ .This extrapolating value is used to determined the so called optical energy gap in amorphous semiconductor .

Fig.(2) shows the relation between $(\alpha h\upsilon)^{1/2}$ and photon energy for Se:2%As thin films deposit at room temperature and annealed to (370,445,520)K. From this figure, it is shown that the value of r=2 , this indicator that indirect transitions are responsible for absorption for all Se:2%As films. The extrapolated value of the indirect energy gap were (1.978,2.082,2.120,2.23) eV at annealing temperature of (295,370,445,520) K respectively.

It is found that the optical gap increases with increasing the annealing temperature. The increasing in annealing temperature changes the density of localized state to a lower values as well as the localized state near the edges. Band gap at high temperature may be related to a decrease the structure defects such as dangling bonds, voids and decrease the disorder of the atomic bonds.

The value of energy gap at room temperature is in agreement with Nang et.al.[15] but it's disagreement with Choudhuri et.al.[16] which they found that the optical energy gap decrease with heat treatment.

Exponential Absorption Edge:

There is an absorption tails at energies smaller than optical energy gap which is called Urbach energy and the absorption coefficient exhibits an exponential behavior. The Urbach energy gives information about localized state in the band gap.

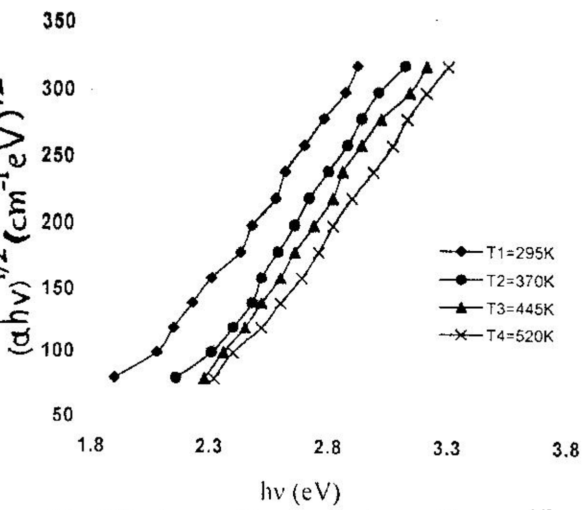

Fig.(2) shows the variation of($\alpha h\nu)^{1/2}$ with photon energy for Se:2%As films at different annealing temperature.

The eq. (2) is employed to evaluated Urbah energy via plot of Ln α against photon energy of Se:2%As films deposited at room temperature and this is shown in Fig.(3) . The reciprocal of the slope of the curve give the value of corresponding ΔE (0.50, 0.42 , 0.31, 0.26) eV at annealing temperature (295,370,445.520)K respectively.

The observed exponential tail of the absorption edge is similar observed by Lanyon [17] has explained the exponential tail in amorphous Se films as due to the exponential distribution of the density of state in the tail region of the valance band .

The band tailing is a function of structural defects, therefore it decrease with increasing the annealing temperature as shown in Fig.(4) .

Conclusion:

1. Thin films samples are amorphous as related by x-ray diffraction.
2. The optical transmission and absorption of Se:2%AS films with thickness of 300 nm have been measured in order to drive data on the absorption edge and band tailing .
3. We found indirect energy gap .
4. The E_{opt} for Se:2%As films showed an increase from a value of 1.978eV at room temperature to 2.23eV at 520K,

while ΔE showed to decrease with increasing the annealing temperature.

5. These results may be related to decrease in voids and dangling bonds.

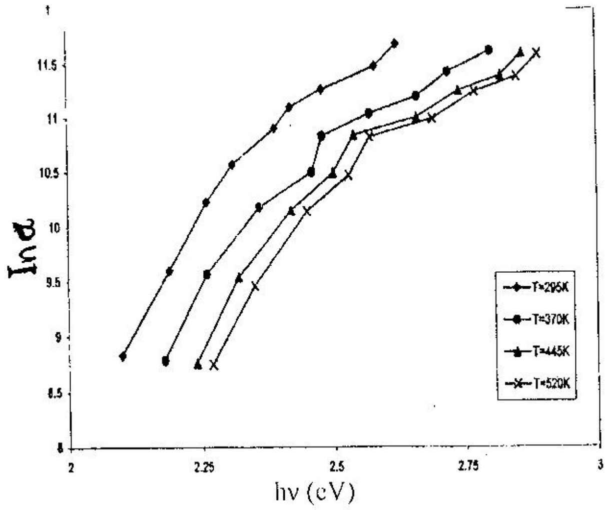

Fig.(3) Shows the variation of lnα with the photon energy for Se:2%As films at different annealing temperature.

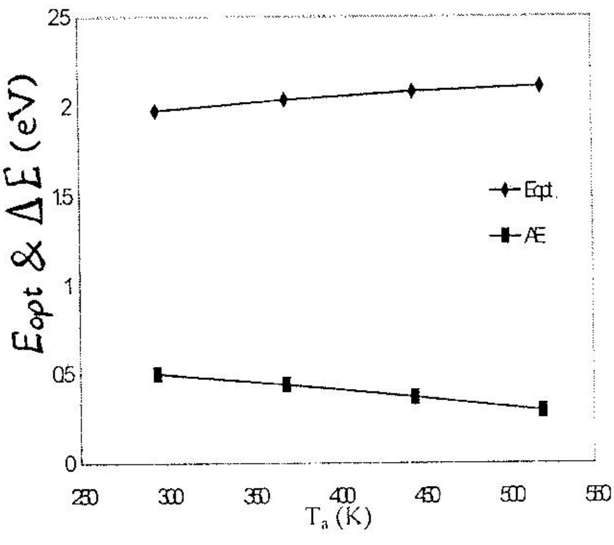

Fig.(4) Shows the value of E_{opt} and bond tailing ΔE with annealing temperature of Se:2%As films.

Table(1) shows the values of E_{opt} and ΔE for Se:2%As films annealed at different temperature .

Annealing temperature T (K)	E_{opt} (eV)
295	1.978
370	2.082
445	2.120
520	2.230

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دراسة درجة حرارة التلدين على الخواص البصرية لأغشية Se:2%As الرقيقة

غصون حميد محمد*

* قسم الفيزياء/كلية العلوم /جامعة بغداد

الخلاصة:

تم دراسة فجوة الطاقة البصرية وعرض الذيول لأغشية Se:2%As المحضرة بطريقة التبخير الحراري في الفراغ كدالة لدرجة حرارة التلدين ضمن مدى طاقة الفوتون eV (1-5.4) . لقد وجد أن لأغشية Se:2%As فجوة للطاقة غير مباشرة وبقيم eV (1.978 , 2.082 , 2.120 , 2.230) عند درجات التلدين K(295,370,445,520) على التوالي . (E_{opt}) و(ΔE) لأغشية Se:2%As كدالة لدرجة حرارة التلدين اظهر زيادة في فجوة الطاقة البصرية وتناقص في عرض الذيول مع درجة الحرارة هذا السلوك قد يعود إلى عيوب التركيب والأواصر المتدلية.اظهر معامل الامتصاص لأغشية Se:2%As اعتماده الأسى على طاقة الفوتون.