The role of annealing temperature on the optical energy gap and Urbach energy of Se:2%Sb thin films

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Abstract:

The optical energy gap(E_{opt}) and the width of the tails of localized states in the band gap (ΔE) for Se:2%Sb thin films prepared by thermal co-evaporation method as a function of annealing temperature are studied in the photon energy range (1 to 5.4)eV.Se2%Sb film was found to be indirect transition with energy gap of (1.973,2.077, 2.096, 2.17) eV at annealing temperature (295,370,445,520)K respectively.

The E_{opt} and ΔE of Se:2%Sb films as a function of annealing temperature showed an increase in E_{opt} and a decrease in ΔE with increasing the annealing temperature. This behavior may be related to structural defects and dangling bonds.

Introduction:

Optical properties of thin films depend mainly on their volume and surface structures[1-2].Film structure is affected by its thickness, conditions of preparation, films material,substrate bulk material and its treatment after preparation [3-5].In recent years,the optical memory effects in amorphous semiconducting films have been investigated and utilized for various device applications[6].

The optical absorption coefficient for many amorphous and glassy materials is found to obey the relation:

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

where υ is the frequency of the incident radiation, β is a constant which depends on density of state of conduction and valence bands, r is a constant depend on the nature of the transition and Eopt is the optical energy gap.

The relation was first derived by Tauc and Colleagues[1] 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[7] obtained the same relation. The width of the tails of localized states at the band edges can be estimated using the Urbach relation[8]:

$$\alpha =\alpha_0 \exp(h\upsilon/\Delta E) \quad \text{…………….(2)}$$

where α_o 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%Sb amorphous thin films at different annealing temperature (295,370,445&520)K.

Experiment:

The purity of the materials are (99.999% pure), 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 306 coating unit.The thickness of films was (~300±5)nm measured using Tolonsky methods.

The glassy nature of the samples were investigated using X-Ray diffraction. Spectral characteristics in the wavelength rang (200-1100)nm were measured using UV-visible recording spectrophotometer(UV-160 Schematize). The absorption coefficient(α) calculated from the relation [9]:

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α =2·303 (A/t) …………….(3)
where A is the absorbance and t is the thickness of the films. The optical band gap calculated from the intercept of $(\alpha h\upsilon)^{1/2}$ data plotted as function of photon energy.

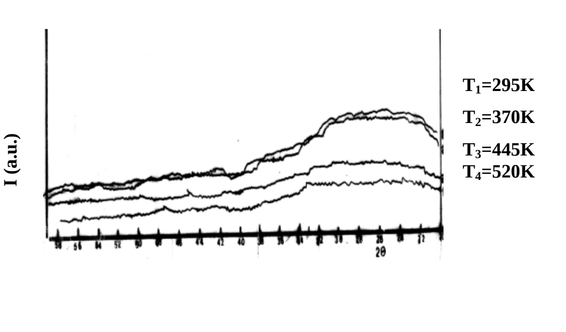
Results and discussions:

The films samples unannealed and annealed at various temperature were amorphous which are conformed by X-ray diffraction as shown in fig. (1). Fig.(2) shows the plots of absorption coefficient (α) versus photon energy (hυ) at different annealing temperature. As evident from Fig.(2), α varies exponentially with hυ in the measured range of α. The absorption edge at room temperature is in a good agreement with the result on Se:2%Sb glass reported by Al-Ani et.al.[10,11].Fig.(3) show plots $(\alpha h\upsilon)^{1/2}$against photon energy of Se:2%Sb films deposit at room temperature and annealed to (370,445,520)K. Fig.(4) shows the plot of ln α against photon energy of Se:2%Sb films deposited at room temperature. The reciprocal of the slope of curve give the value of corresponding ΔE (0.45, 0.38, 0.29, 0.23) eV at annealing temperature (295,370,445.520)K respectively The extrapolated value of the indirect energy gap were (1.973,2.077,2.096,2.17)eV at annealing temperature of (295,370,445,520)K respectively as shown in Fig.(5) which is shows the variation of E_{opt} and ΔE with T. The value of energy gap at room temperature is in agreement with Nang et.al.[12] but it´s disagree with Choudhuri et. al.[13] which they found that the optical energy gap decrease with heat treatment.

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 band tailing is a function of structural defects, therefor it decrease with increasing the annealing temperature as shown in Fig.(5).

Conclusion:

The optical transmission of Se:2%Sb films with thicknesses of 300 nm have been measured in order to drive data on the absorption edge and band tailing . They found to be a indirect energy gap. The E_{opt} for Se:2%Sb films showed an increase from a value of 1.978eV at room temperature to 2.17eV at 520K. While ΔE showed to be decreases with increasing the annealing temperature. These results may be related to a decrease in voids and dangling bonds.



Fig(1): XRD Patterns of Se:2%Sb thin films

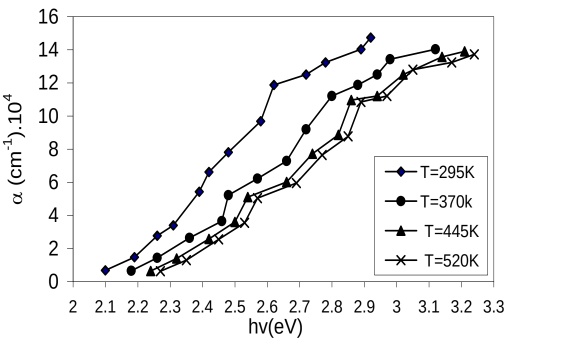
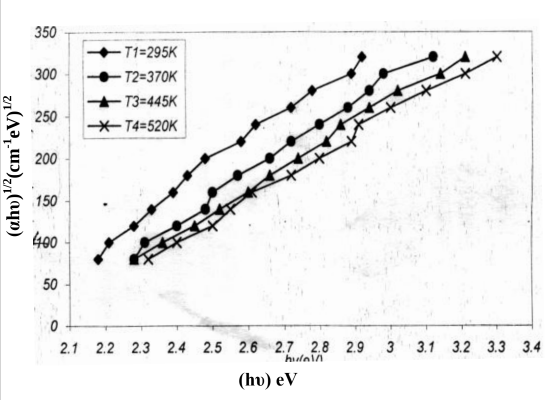


Fig.2: α against photon energy of Se:2%Sb films at different annealing temp.



Fig(3): $(\alpha h\upsilon)^{1/2}$ against photon energy of Se:2%Sb films at different annealing temperatures

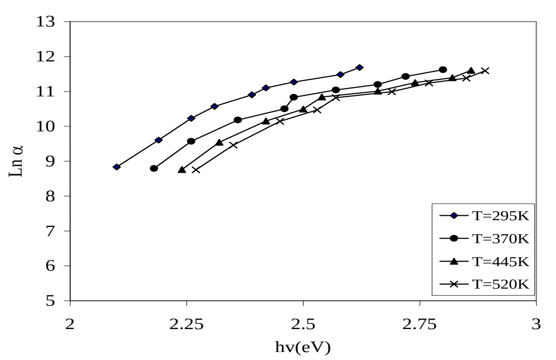


Fig.(4):Lnα against photon energy of Se:2%Sb films at different annealing temperature.

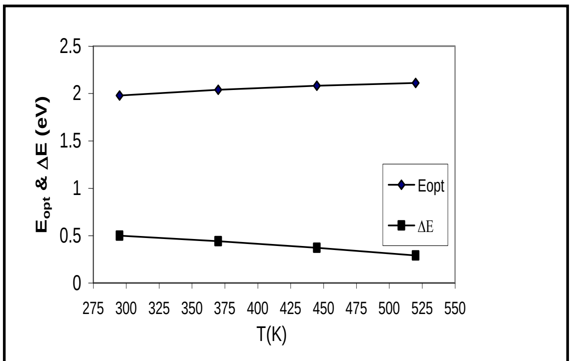


Fig.(5):Variation of Eopt and ΔE against annealing temperatures of Se:2%Sb films.

References:

1. Saad, M.M., A.A.Saad,A.M.Elhelou, S.M.Botors,1988,Optical properties of selenium thin films,OpticaApplicata. 17(2):.105.
2. Al-Ani, S.K.,M.N.Makadsi, N.K. Abass.,2005,"Structural studies of the Ge-Se-Bisystem"J.of Natural and Applied Sciences, 9(2):399.
3. Abbas, L.K.,2003,The study of the effect of annealingtemperature onthe optical properties of Ge-Se semicond. ,J.ofCollege of Education, 12(2):372.
4. Chadhi,S.,S.Biswas,1981, Amorphous to crystallian Transition of selenium thin films of different thickness, JNon- Cryst. Solid, 4(171) : 171.
5. Twaddeii,V.A.,W.C.Lacourse.,andJ.D .Mackenzie,1972,"Impurity effects on the structure and electrical properties of non-crystalline selenium"J.of Non-crystalline Solids, 8(10):p.189.
6. Khan,Z.H.,M.Zulfeqaur,andM.Husain, 2002,Electricalconductivity and thermoelectric power of a-$Se_{80-x}In_x$ and $Se_{80-x}Ge_{20}In_x$ thin films."Canda J. Phys.10.
7. Davis, E., N.Mott,1979,Electronic process in Non-crystallian materials 2nd ed.,Claredon Press.Oxford.
8. Ihm J.,1985,.Urbach tails and the structure of chalcogenide Glasses. 53(3):293.
9. Jenkins, F.,H. White, 1957,. Fundamentals of optics.,3rd ed.,Mc Graws-Hill Book Company,New York.
10. Al-Ani,S.KM.N. Makadsi,L.K. Abbas, 1999, The effect of some additives on optical properties of a-Se thin films,Second Scientific Conference/ College of Scince/University of Baghdad.
11. Al-Ani,S.K.J., 1984,.Studiesof Optical and related Properties ofThin Amorphuos film. Ph.D.Thesis, Brunel University, England.
12. Nang,T.T.,M. OkudaM.,1979, Cmpositionnn dependenc of the rrefractive index and its photon energy variation in the system e-Se andAs-Se,J.of Non Cryst. Solid,33 (311):311-322.

13. Chaudhuri ,S.,S. Biswas, 1983, Variation of optical ofamorphous selenium film on heat treatment,J.Non-Cryst.Solids, 54:179-182.

تأثير درجة حرارة التلدين على فجوة الطاقة البصرية وطاقة اورباخ لأغشية Se:2%Sb

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الخلاصة:

تم دراسة فجوة الطاقة البصرية وعرض الذيول للمستويات الموضعية لأغشية Se:2%Sb المحضرة بطريقة التبخير الحراري المزدوج كدالة لدرجة حرارة التلدين ضمن مدى طاقة الفوتون (1-5.4) eV.

لقدوجد ان لاغشية Se:2%Sb فجوة للطاقة غيرمباشرةوبقيم(2.17,2.096,2.077,1.973) eV عند درجات التلدين (520,445,370,295)K على التوالي.ان فجوة الطاقةالبصرية وعرض الذيول للمستويات الموضعية (E_{opt}) و(ΔE) لاغشية Se:2%Sb كدالة لدرجة حرارة التلدين اظهر زيادة في فجوة الطاقة البصرية وتنا قص في عرض الذيول مع درجة الحرارة. هذا السلوك قد يعود الى عيوب التركيب والاواصر المتدلية.