

PAPER • OPEN ACCESS

Studying the effect of doping by Ag on the structural and optical properties of a-As₂Te₃ thin films

To cite this article: Yusif. H. Sheban *et al* 2020 *IOP Conf. Ser.: Mater. Sci. Eng.* **928** 072129

View the [article online](#) for updates and enhancements.

You may also like

- [Pressure-induced phase transition in magnetoresistance perovskite La_{0.75}Ca_{0.25}MnO₃: a GGA + U study](#)
D P Mankou Bakala, L Mouketo, B R Malonda-Boungou et al.
- [Proposal of an analytical method based on linear regression for modeling reliability by Weibull law](#)
A Boroiu, V Nicolae, O Alssadi et al.
- [VLA AND CARMA OBSERVATIONS OF PROTOSTARS IN THE CEPHEUS CLOUDS: SUB-ARCSECOND PROTO-BINARIES FORMED VIA DISK FRAGMENTATION](#)
John J. Tobin, Claire J. Chandler, David J. Wilner et al.



ECS
The
Electrochemical
Society
Advancing solid state &
electrochemical science & technology

DISCOVER
how sustainability
intersects with
electrochemistry & solid
state science research

Studying the effect of doping by Ag on the structural and optical properties of a-As₂Te₃ thin films

Yusif .H.Sheban ⁽¹⁾, Aliyah.A.Shihab⁽²⁾, Najat.A.Dahham⁽¹⁾

1- Department of physics, college of science ,Tikrit University

2- Department of physics, college of Education of pure science (Ibn AL-Haitham)/university of Baghdad

dr.najat1970@gmail.com

Abstract

a-As₂Te₃ was made of high purity elements that were productive. Thin film at a thickness (400 nm) was prepared using thermal evaporation techniques on cleaned glass substrates under very low vacuum (2×10^{-5} mbar) with precipitation rate (0.33nm/s). The X-ray diffractometer showed that the pure film structure was amorphous, and the doping sample structure as polycrystalline. The result of optical properties has shown that pure and doping films have allowed a direct optical energy gap, and the energy gap for the pure film is (1.25eV) and decreases whenever we add impurities.

Keywords: a-As₂Te₃ thin film; optical properties; amorphous chalcogenides

1-Introduction

Chalcogenides are materials that mostly contain one of the chalcogen elements (e.g. S, Se or Te) and one or more metallic ions from group IVA and VA. Chalcogenides are covalently bound materials and can be amorphous or crystalline with usually 1-3 eV band gaps. Chalcogenide glasses or crystals are somewhat distinct from conventional glasses, silica or silicates with a much wider range of approximately 8 eV band gaps [1].

Chalcogenide based on tellurium is thought to be suitable for use in IR photonics and optoelectronics [2, 8] also for the development of the three-dimensional architecture of integrated optical elements of future quantum computers [8, 10]. The effect of adjusting the threshold for the telluride glass Pearson and Northover was first observed in the 1960 s [11, 12].

The a-Se, a-As₂Se₃ and a-As₂Te₃ Chalcogenide glass Its technological applications were of great interest Which include photovoltaic cells, grinders, optical recording, Fibers optics, xerography, memory and switching Apparatus [13, 18]. a-As₂Te₃ intergroup compound (VI) to (V) element has a very high conductivity and simple band structure[19].

Many researchers studied a- As₂Te₃ film and bulk structural and optical properties; p.hawlova et al [20] The structure and optical properties of a-As₂Te₃ were studied using a pulsed laser deposition technique and demonstrated that the XRD for a-As₂Te₃ thin film is amorphous and found that the energy gap is (0.9ev); scheidmatel et al [21,22] The pressure-induced structural phase transition from a-As₂Te₃ (monoclinic) to B-As₂Te₃ (rhombohedral) near 7Gpa was revealed, resulting in a dramatic increase in thermoelectric power; Studies of the mechanical reaction, dynamic/thermal



stability, electronic/optical properties and monoclinic photocatalytic characteristics for a-As₂Te₃; leoid mochalov et al [23] Studied AS₂Te₃ thin-film structure and optical properties prepared by PECVD using various chemical and phase composition; Abear M.M.Ali et al [24] The structure and optoelectronic properties of a-As₂Te₃ thin film prepared by thermal vacuum evaporation at different thicknesses (200,250,300,350)nm were studied; the structural properties were amorphous for all thicknesses and the energy gap was indirectly allowed to transition its value to the thickness (0,8,0,77,0,72,0,66)eV[24].

The aim of this systematic work is to research the structure and optical properties of thin-film a-As₂Te₃ prepared by thermal vacuum evaporation at a doping thickness (400 nm) by Ag.

2-Experimental and details

a-As₂Te₃ thin film was prepared at thickness (400)nm on cleaned glass substrates using thermal vacuum evaporation technique (using Edward modal (E306)) coating unit under deflated (2.5×10^{-5}) mbar.

Ag Impurities a-As₂Te₃ thin film with specific impurity ratios (2,3and4) % are prepared by thermal diffusion, if thin films of a-As₂Te₃ are put on top of the basin in which the material Ag is contained and which achieves one of the following weight ratios (2, 3, and 4) % when sedimentation is done after heating the substrate to a temperature (200C°) and then after evaporation.

Structural measurement using a model of x-ray diffractometer (Shimadzu lab XRD6000) the device specifications copper $k\alpha$ wavelength radiation ($\lambda = 1.5406 \text{ \AA}$) with voltages (40k volts) to find the structural thin film.

The optical absorption (A) and transmittances (T) of the thin film layer is measured at a standard incidence at room temperature using a double UV-vis scanning spectrophotometer (Biotech UV-vis 1800 spectrophotometer) at the wavelength range of (300-1100 nm).

The absorption coefficient (α) is defined as the ratio of attenuation in the intensity of incident radiation per unit area toward the wave propagation within the medium. It depends on the energy of the incident photon and the properties of the semiconductor including the energy gap, optical transmission, and the type of optical transition [25]

The following equation below refers to the coefficient of absorption [25]:

$$\alpha = 2.303 \frac{A}{t} \quad (1)$$

Where: A: optical absorbance, t: film thickness

The absorption equation in semiconductors that give a direct energy gap (E_g) is given by the following relationship [25] :

$$\alpha h\nu = B(h\nu - E_g)^r \quad (2)$$

B: is a constant , Depending on the form of transition , the exponent r has several values (2,3,3/2,1/2) corresponding to allowed direct , forbidden indirect transition ,allowed in direct , forbidden direct and allowed direct ,respectively and $h\nu$ is photon energy incident , which calculated from this formula :

$$h\nu \text{ (eV)} = \frac{1240}{\lambda \text{ (nm)}} \quad (3)$$

3-Result and discussion

3-1 Structure properties

Figure (1) shows the result of the measurement of x-ray diffraction (XRD) for (a-As₂Te₃) thin film, that appears the narrow of the x-ray as it shows in figure(1-a) the pure thin film in (RT) was (amorphous) structure and the result is similar to the researcher [24] and after silver doping, with (2,3 and 4) % the crystal structure turned into polycrystalline Where the figures(1-b,c,d) are shown appears of four peaks (40,1), (112), (311), (403) it represents the phase of the monoclinic system for the (a-As₂Te₃) films when compared with American standards testing materials (ASTM)(00-015-0407) and we note to the appears of the fifth peak for all doping ratios represent this peak The silver cubic phase when compared with the (ASTM) (00-003-0931), which are shown in figure (1) the distress changes from one percent to another but it decreases that on the (ASTM) And the reason for it is the entry of the (Ag) atoms in the crystal structure of the (a-As₂Te₃) film.

It has been calculating grain size (D) for pure and doping thin film by using Scherer's formula []

$$D = \frac{k\lambda}{\beta' \cos\theta} \quad (4)$$

Where D: grain size , k: is some constant 0.9 for a-As₂Te₃

B: the angular line width of half maximum intensity, θ : is the Bragg's diffraction angle

we note from the table (1) that doping leads to increasing the width of the band in the middle of the intensity (FWHM) and therefore decreasing in the grain size the reason for this decrease is the amount of difference in the ionic diameter size for the tellurium ionic (Te⁻²) whose amount is (2.07Å) while the ionic diameter for the (Ag⁺²) is (1.09Å) so it's allowing the (Ag) atoms to occupy the interstitial cations in crystal structure for the tellurium which works in turn on the decreases the interstitial crystal cations, therefore, decreases the grain size and also the changes in the peaks sites.

Table (1) the structural parameters for a-As₂Te₃ film pure with different doping ratios

Ratio	2 θ (deg)	(hkl)	d(Å)	FWHM (deg)	FWHM(β) (RAD)	D(nm)
ASTM	27.4202	(401)	3.2500			
	29.7559	(112)	3.000			
	31.137	(311)	2.8700			
	38.8522	(403)	2.3160			
	44.1409	(200)	2.0500			
Ag2%	26.6881	(401)	3.3375	0.2800	0.004884	39.8268

	28.8449	(112)	3.0922	0.4134	0.007212	68.2870
	30.8273	(311)	2.898	0.3700	0.006454	22.4399
	38.7078	(403)	2.3243	0.4060	0.007082	22.3540
	44.1828	(200)	2.0482	0.5967	0.010409	13.3825
Ag3%	26.6115	(401)	3.3469	0.2467	0.004304	38.4069
	28.8948	(112)	3.0874	0.2900	0.005059	62.9518
	30.8423	(311)	2.8968	0.2266	0.003953	22.38966
	38.7198	(403)	2.3267	0.2266	0.003953	22.4286
	44.1512	(200)	2.0496	0.3466	0.006046	13.3630
Ag4%	26.5649	(401)	3.3527	0.3667	0.006397	37.6178
	28.8529	(112)	3.0918	0.3360	0.005861	67.3687
	30.7457	(311)	2.9057	0.4467	0.007792	22.7400
	38.7098	(403)	2.3242	0.4100	0.007152	22.3663
	44.0863	(200)	2.0524	0.4700	0.008199	13.3334

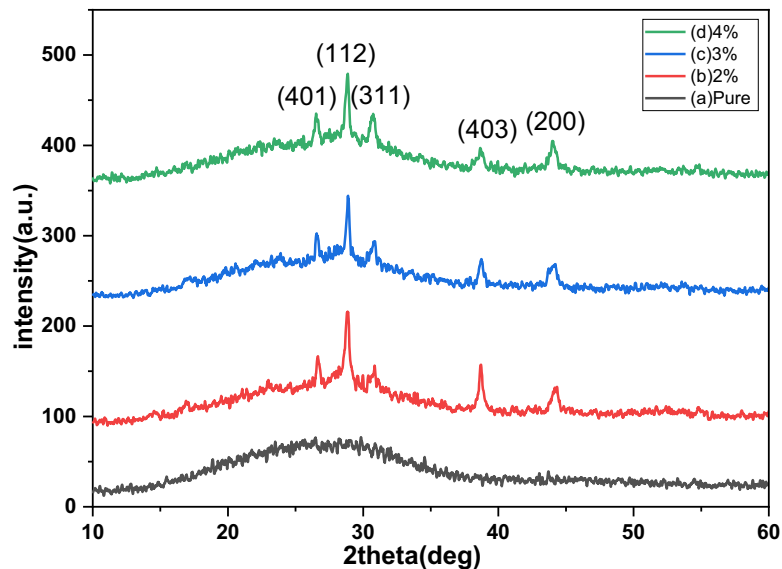


Figure (1) x-ray diffraction pattern of a- As_2Te_3 with different ratio doping by Ag

3-2 optical properties

In order to figure out the optical properties of thin-film and whether it can be used in research applications, you will analyze these features, such as the absorbance spectrum, which relies on film

materials, the crystal structure, in addition to the energy photon events on the glass, which this spectrum considers to be a distinctive characteristic of the materials. [26]

The film absorbance spectrum with a wavelength range between (300-1100) nm was studied. The results showed a large decreases in absorbance with an increasing in doping ratio for (Ag) as shown in Figure (2) because (Ag) has greater transparency of arsenic telluride so that it forms a dark layer on the film surface and the doping process, produces more levels below the conduction band so it decreases the possibility of photon absorbs and whose increase the process of electronic transmission from valance band into energy gap during the conduction band.

It notices that the absorption is less if the film impurity as it reaches the absorbance (3.4) and decreases the more it increases the wavelength while on the doping film it reaches (2.6) where it increases when the wavelength is greater to reach the highest peak when the wavelength between (450-750) nm is between the visible spectrum so this thing referred to the possibility of using the films in Photoelectric cells.

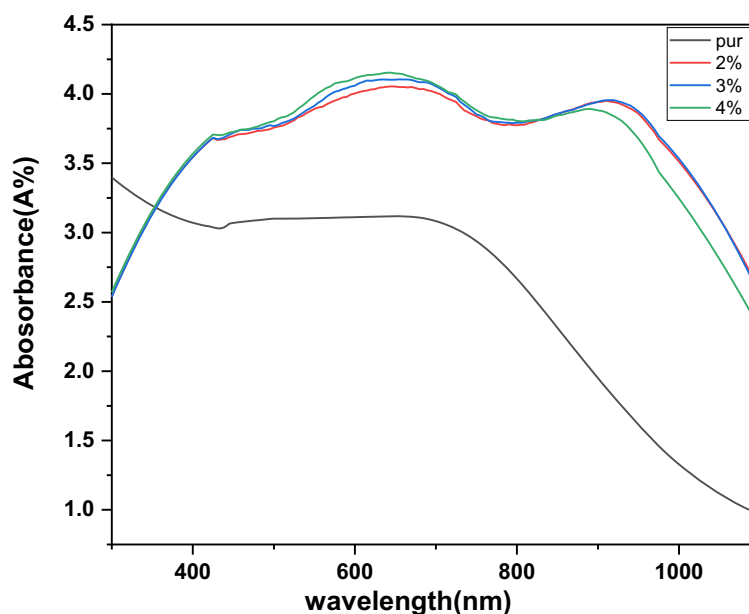


Figure (2) absorbance spectrum for (a-As₂Te₃) thin film at doping by Ag

Figure (3) shows the film's transmittance spectrum as the function of the wavelength that produces from deposition. We note from the transmittance for all films there are few in the visible spectrum area and the reason for it is the increasing the absorbance of the light and this property suitable in photoelectric cells Application.

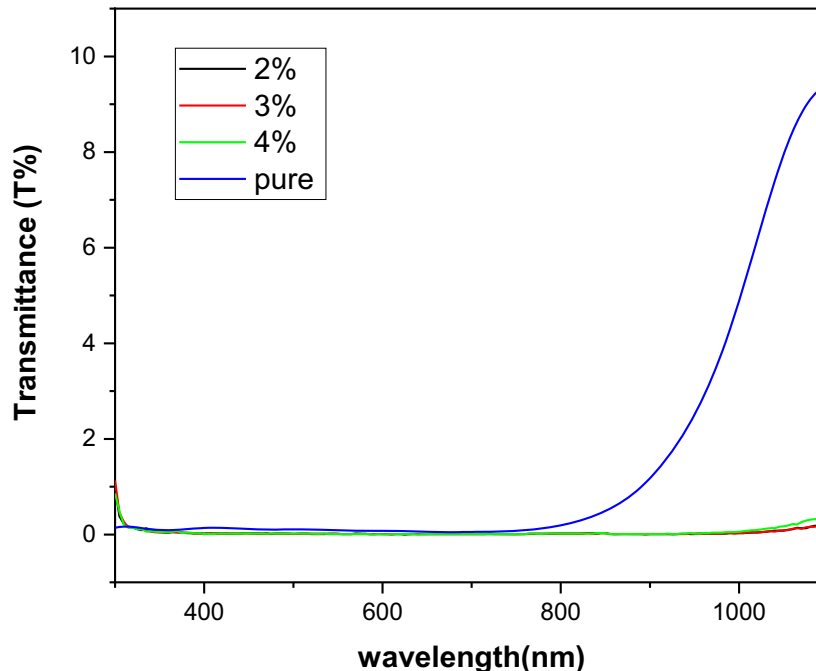


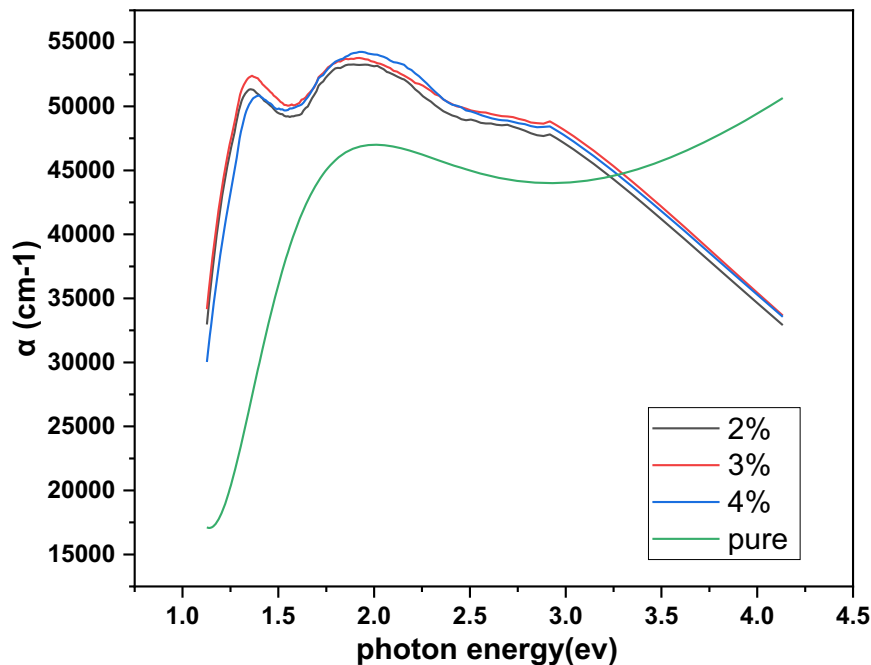
Figure (3) Transmittance spectra for (a-As₂Te₃) thin film at different doping by Ag

We conclude from the transmittance spectrum that the pure film has high transmittance in the near-infrared (IR) region of the electromagnetic spectrum.

Figure (4) absorption coefficient (α) of films. Note from the figure that the optical absorption coefficient (α) begins to change as a function of the photon energy ($h\nu$).

It is noted that the absorption coefficient is higher than $\alpha \geq 10^4 \text{ cm}^{-1}$, and this refers that these films may have allowed direct transition.

The absorption coefficient (α) increases with the increase in photon energy ($h\nu$) within the energy band (1.2-3) eV, where it increases with increasing impurity ratios where its highest values in the energy band (1.4-2.25) eV reach its highest value at the impurity rate (4%). The reason for this is that the impurity atoms helped in the formation of the positional levels that help to increase the absorbance and thus increasing the absorption coefficient because the proportion between them is directly proportional according to the formula (1).



Figure(4) changes of absorption coefficient with wavelength for a-As₂Te₃ thin film at different doping by Ag

It has been calculated the direct energy optical gap from formula (2) and since the value of (α) is greater than or equal to ($\alpha \geq 10^{-4} \text{ cm}^{-1}$) for all the films, so the value of (r) in the formula (2) is the ($\frac{1}{2}$) to the direct allowed transition .

The value of the energy gap E_g from the graph formula between the incident energy photon ($h\nu$) on the x-axis and $(\alpha h\nu)^2$ on the y-axis was defined and stretches from the curve on the straight line. The effect would go through the x-axis ($h\nu$) at a point where the direct optical energy gap for this film is represented ,Figure(5-a) and table(2) represent the energy gap for the pure film not similar to this author[24] because the thickness of the film is varies , Figure 5(b, c, d) and on table (2)represents the value of the impurity film energy gap showing that (E_g) decreases as the impurity ratio of the values increasing (2,3,4) per cent. , and we can clarify this decrease with the enter of the positive (Ag^{+2}) to the crystal structure for the telluride (Te^{-2}) element which generates increasing with the number of the positive ions, so, therefore, will generate internal levels inside the energy gap causes decreasing in its value [27].it's possible to clarify the reason for this decrease is because of the changing of lattice constant [28], this result matches the properties structure.

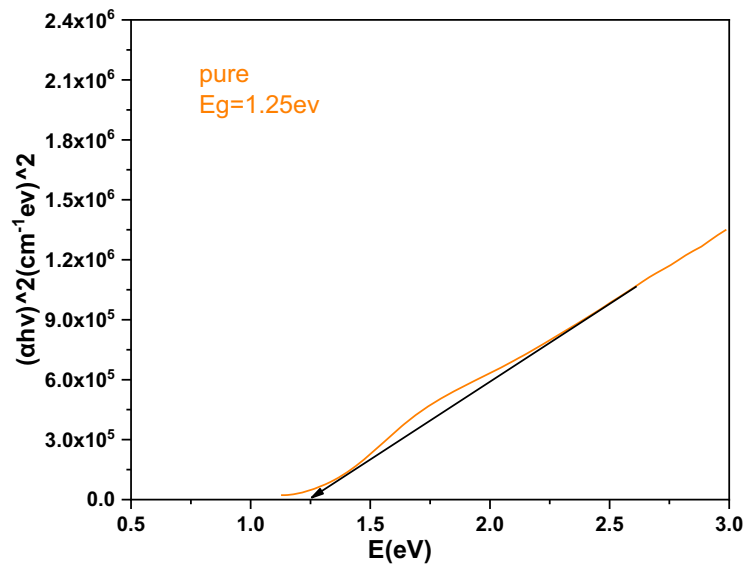


Figure (5-a) shows the energy gap for a-As₂Te₃ pure film

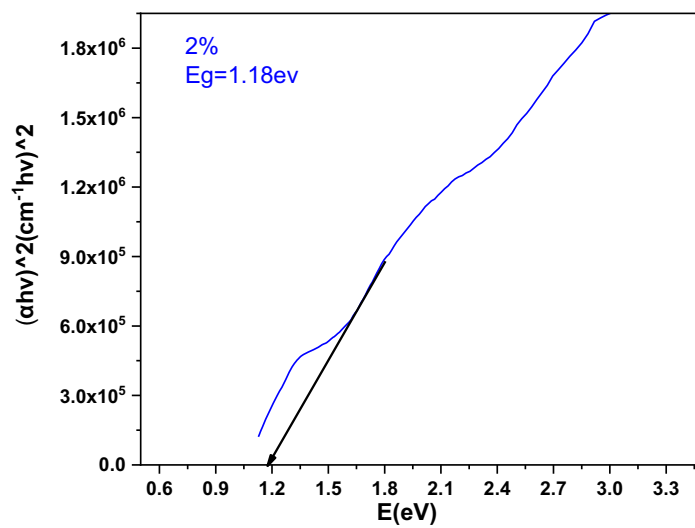


Figure (5-b) shows energy gap for a-As₂Te₃ film doping by Ag

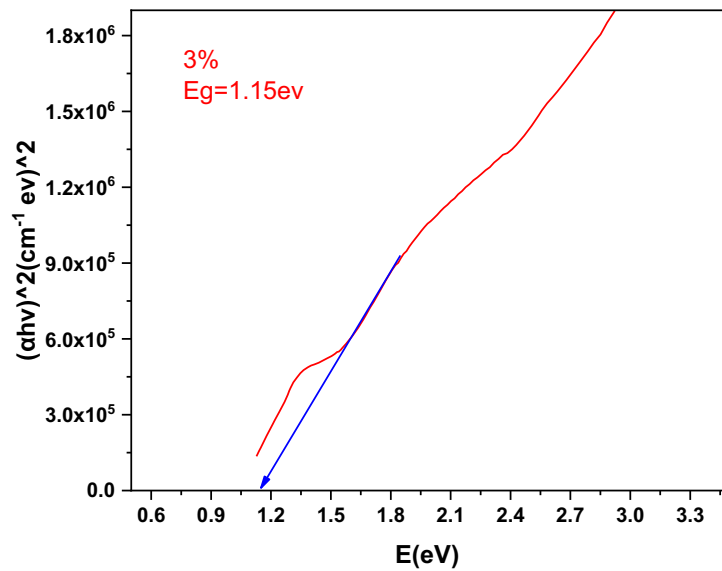


Figure (5-c) shows energy gap for a-As₂Te₃ film doping by 3% Ag

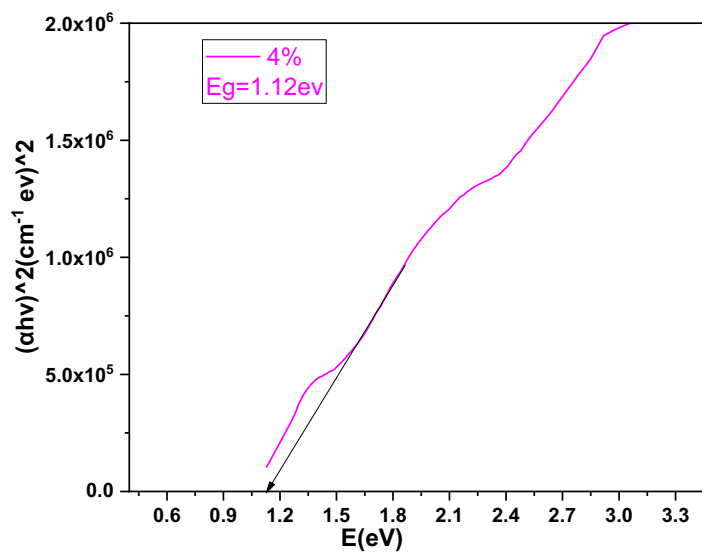


Figure (5-d) shows energy gap for a-As₂Te₃ film doping by 4% Ag

Table (2) energy gap for all the films

Sample	Energy gap (eV)
Pure	1.25eV
2%	1.18eV
3%	1.15eV
4%	1.12eV

Conclusion

the x-ray diffraction measurement show that the crystal structure for the pure film is (amorphous), and when adding (Ag), the crystal structure transforms into polycrystalline and the prevailing direction is (112), the UV-visible measurement shows that the absorbance of the pure film increase when to add impurities of the (Ag) and the absorption coefficient has value was ($\alpha \geq 10^4 \text{ cm}^{-1}$) which refer it has allowed direct energy gap.

References

- [1] Zakery, A. (2007). Optical nonlinearities in chalcogenide glasses and their applications. Springer-Verlag Berlin Heidelberg.
- [2] Mochalov, L.; Dorosz, D.; Nezhdanov, A.; Kudryashov, M.; Zelentsov, S.; Usanov, D. and Gogova, D. (2018). Investigation of the composition-structure-property relationship of $\text{As}_x\text{Te}_{100-x}$ films prepared by plasma deposition. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 191: 211-216.
- [3] Mochalov, L.; Nezhdanov, A.; Strikovskiy, A.; Gushin, M.; Chidichimo, G.; De Filpo, G. and Mashin, A. (2017). Synthesis and properties of $\text{As}_x\text{Te}_{100-x}$ films prepared by plasma deposition via elemental As and Te. *Optical and Quantum Electronics*, 49(8): 274.
- [4] Mochalov, L.; Nezhdanov, A.; Kudryashov, M.; Logunov, A.; Strikovskiy, A.; Gushchin, M. and Mashin, A. (2017). Influence of plasma-enhanced chemical vapor deposition parameters on characteristics of As-Te chalcogenide films. *Plasma Chemistry and Plasma Processing*, 37(5): 1417-1429.
- [5] Mochalov, L.; Nezhdanov, A.; Usanov, D.; Markelov, A.; Trushin, V.; Chidichimo, G. and Mashin, A. (2017). A new method for synthesis of As-Te chalcogenide films. *Superlattices and Microstructures*, 111: 173-180.
- [6] Mochalov, L.; Nezhdanov, A.; Usanov, D.; Markelov, A.; Trushin, V.; Chidichimo, G. and Mashin, A. (2017). A new method for synthesis of As-Te chalcogenide films. *Superlattices and Microstructures*, 111: 173-180.
- [7] Shiryayev, V. S.; Adam, J. L.; Zhang, X. H.; Boussard-Plédel, C.; Lucas, J. and Churbanov, M. F. (2004). Infrared fibers based on Te-As-Se glass system with low optical losses. *Journal of non-crystalline solids*, 336(2): 113-119.
- [8] Nalivaiko, V. I. (2007). Materials for optical information recording on the base of subnanostructured chalcogenide films. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, 575(1-2): 113-115.
- [9] Kolobov, A. V. (Ed.). (2006). Photo-induced metastability in amorphous semiconductors. John Wiley and Sons.
- [10] Efimov, O. M.; Glebov, L. B.; Richardson, K. A.; Van Stryland, E.; Cardinal, T.; Park, S. H. and Bruneel, J. L. (2001). Waveguide writing in chalcogenide glasses by a train of femtosecond laser pulses. *Optical Materials*, 17(3): 379-386.
- [11] Northover, W. R. and Pearson, A. D. (1964). U.S. Patent No. 3,117,013. Washington, DC: U.S. Patent and Trademark Office.
- [12] Dewald, J. F.; Northover, W. R. and Pearson, A. D. (1966). U.S. Patent No. 3,241,009. Washington, DC: U.S. Patent and Trademark Office.
- [13] Fritzsche, H. and Tauc, J. (1974). Amorphous and liquid semiconductors. Plenum Press, New York, 1974) p, 254.
- [14] Elliott, S. R. (1990). *Physics of Amorphous Materials*, Longman. New York.
- [15] Bube, R. H. (1992). *Photoelectronic properties of semiconductors*. Cambridge University Press.
- [16] El-Nahass, M. M.; Ali, M. H.; El-Shazly, E. A. A. and Zedan, I. T. (2016). Junction parameters and characterization of Au/n-Ge 15 In 5 Se 80/p-Si/Al heterojunction. *Applied Physics A*, 122(8): 780.
- [17] Abd-Elrahman, M. I.; Hafiz, M. M.; Qasem, A. and Abdel-Rahim, M. A. (2016). Characterization of the optical constants and dispersion parameters of chalcogenide Te 40 Se 30 S 30 thin film: thickness effect. *Applied Physics A*, 122(2): 45.
- [18] Rao, G. K. (2017). Electrical and photoresponse properties of vacuum deposited Si/Al: ZnSe and Bi: ZnTe/Al: ZnSe photodiodes. *Applied Physics A*, 123(4): 224.
- [19] z.u.Borisoval (1981). *Glassy semiconductors* .by.z.u.Borisova.New York .

- [20] Hawlová, P.; Bouška, M.; Nazabal, V.; Baudet, E.; Černošek, Z. and Němec, P. (2017). Photostability of pulsed-laser-deposited $\text{As}_x\text{Te}_{100-x}$ ($x = 40, 50, 60$) amorphous thin films. *Optics Letters*, 42(9): 1660-1663.
- [21] Scheidemantel, T. J.; Meng, J. F. and Badding, J. V. (2005). Thermoelectric power and phase transition of polycrystalline As_2Te_3 under pressure. *Journal of Physics and Chemistry of Solids*, 66(10): 1744-1747.
- [22] Scheidemantel, T. J. and Badding, J. V. (2003). Electronic structure of $\beta\text{-As}_2\text{Te}_3$. *Solid state communications*, 127(9-10): 667-670.
- [23] Mochalov, L.; Logunov, A.; Markin, A.; Kitnis, A. and Vorotyntsev, V. (2020). Plasma-prepared arsenic telluride films: relationship between physico-chemical properties on the parameters of the deposition process. *Materials Research Express*, 6(12): 126436.
- [24] Abear, M. M.; Alia, A. S. and H. K. Alamy, (2001). study the structure and optoelectronic for $\alpha\text{-As}_2\text{Te}_3$ thin film, university of Baghdad, department of physics.
- [25] Vilaplana, R.; Gomis, O.; Manjón, F. J.; Segura, A.; Pérez-González, E.; Rodríguez-Hernández, P. and Drasar, C. (2011). High-pressure vibrational and optical study of Bi_2Te_3 . *Physical Review B*, 84(10): 104112.
- [26] Yang, Z. X.; Zhong, W.; Yin, Y. X.; Du, X.; Deng, Y.; Au, C. and Du, Y. W. (2010). Controllable synthesis of single-crystalline CdO and $\text{Cd}(\text{OH})_2$ nanowires by a simple hydrothermal approach. *Nanoscale Research Letters*, 5(6): 961-965.
- [27] Xu, B.; Choi, J.; Caruso, A. N. and Dowben, P. A. (2002). Band filling and depletion through the doping of polyaniline thin films. *Applied physics letters*, 80(23): 4342-4344.
- [28] Ayush Khare and Slashi Bhushan, "Electroluminescence studies of Chemically deposited (Zn-Cd)S Cu, films", *Crystal Res Technol.* 41, No. 7, (2006) pp 689