# Preparation and analysis of Ag<sub>2</sub>Se<sub>1-x</sub>Te <sub>x</sub> thin film structure on the physical properties at various temperatures by thermal evaporation

Hiba M. Ali<sup>\*</sup>, I. Khudayer

Department of Physics, College of Education for Pure Science / Ibn Al-Haitham, University of Baghdad, Baghdad, Iraq

Silver selenide telluride Semiconducting  $(Ag_2Se_{0.8}Te_{0.2})$  thin films were by thermal evaporation at RT with thickness350 nm at annealing temperatures (300, 348, 398, and 448) °K for 1 hour on glass substrates .using X-ray diffraction, the structural characteristics were calculated as a function of annealing temperatures with no preferential orientation along any plane. Atomic force microscopy (AFM) and X-ray techniques are used to analyze the Ag\_2SeTe thin films' physical makeup and properties. AFM techniques were used to analyze the surface morphology of the Ag\_2SeTe films, and the results showed that the values for average diameter, surface roughness, and grain size mutation increased with annealing temperature (116.36-171.02) nm The transmittance and absorbance spectra are also analyzed and published in accordance with the wavelength range of (400-1100) nm, The results show that the sample's maximum absorbance value was obtained at a temperature treatment of 448 K, The findings show that the thin films under study are particular of direct transitions at optical energies of 2.05& 1.7& 1.65 and 1.6 ev.

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# 1. Introduction

Interesting semiconducting ternary systems like Ag2SeTe may find use in things like magneto-optic sensors, energy storage devices, and photosensitizers. [1-2] Because of their unique optical and optoelectronic characteristics, metal selenides have gained a lot of attention in recent years. These qualities have led to some good applications, including super-ionic conductors, solar cells, thermochromic materials, and photosensitizers [3]. The optical properties of chalcogenide glassy semiconductors are changed by the presence of impurity atoms in binary Se-Te systems, according to experimental findings published by numerous researchers. Glass science and technology have shown a great deal of interest in studying the structure, characteristics, and manufacture of chalcogenide glasses that contain silver. Numerous intriguing and practical electrical characteristics are displayed by silver selenide[4]. In specifically, the structural phase shift takes place when the temperature rises. Silver selenide has two different phases that depend on temperature: has an orthorhombic structure, while the high-temperature phase  $\beta$  -Ag2Se, has a bcc structure. With a transition temperature of roughly 408 K or 395 K, silver selenide exists as a high-temperature cubic phase (a)The low temperature phase and the high temperature phase are separated by a transition temperature of 130 °C. The latter, a semiconductor with a small bandgap, has been widely used as a photosensitizer in photographic films or as a thermo chromic material. In photo chargeable secondary batteries, the former, Ag2Se, is employed as the solid electrolyte. It is a supersonic conductor. Silver selenide is a compound semiconductor belonging to the BIV group with a high Seebeck coefficient, great electrical conductivity, and extremely low lattice thermal conductivity. This solid's nonstoichiometric derivative has also been linked to a substantial magneto resistance, according to recent investigations a nonstoichiometric derivative of this solid has also been linked to a considerable magneto resistance. [5–6]. For sensing devices, especially low field sensors, the characteristic of linear dependency on the magnetic field is used. The manufacture of I-IV compound nanostructured materials has been the subject of several studies.

<sup>\*</sup> Corresponding author : hiba.m.a@ihcoedu.uobaghdad.edu.iq https://doi.org/10.15251/CL.2023.203.197

[7] The fabrication of highly ordered, stoichiometric Ag2Se and ternary Ag<sub>2</sub>Se1-xTex nanowire arrays from nonaqueous dimethyl sulfide oxide solutions has been described as a unique electrochemical method. Through the low-temperature thermal reaction of silver carbonate and selenium, crystalline Ag<sub>2</sub>Se in various forms [8] was created. Orthorhombic  $\beta$ -Ag<sub>2</sub>Se thin film was fabricated by pulsed-laser deposition method [9-10] Studies on Ag<sub>2</sub>Te are very intriguing because, to our knowledge, there hasn't been a thorough analysis of the silver selenide telluride (Ag<sub>2</sub>SeTe) ternary system in the literature. In this study, we used the thermal evaporation approach to create the ternary complex  $Ag_2Se_{1-x}Te_x$ , which is a great way to create these kinds of thin film ternary compounds since it allows for process control. Using X-ray diffraction (XRD) and optical absorption methods, the structural and optical characteristics of the produced thin films were investigated. Calculations are made for optical constants such as optical conductivity, the imaginary and real components of the dielectric constant, the absorption coefficient, and the optical band gap [11–12]. A number of different types of crystalline b-Ag<sub>2</sub>Se have been produced via thermal evaporation. In this case, we experimented with a method that had received little prior study. Here, we discuss the structural and optical properties of an Ag<sub>2</sub>Se<sub>0.8</sub>Te<sub>0.2</sub> thin film produced by thermal evaporation. [13-14]

# 2. Experimental

To produce thin films of Ag2Se0.8Te0.2 powder in this investigation, alloy silver selenide telluride was used (99.99 percent, 99.5 percent). A quartz tube that had been evacuated was used to make the alloy. The alloy (3g) thin films were made using (E 306) thermal evaporation at RT deposited on glass substrates with 350 nm thickness, then vacuum annealing temperatures (348, 398, and 448) K, which were created on glass substrates in a high vacuum utilizing the thermal evaporation process on one type of substrate (glass slides). [14] Thermal evaporation techniques were used to create the thin films. When an X-ray diffract meter (SHIMADZU Japan XRD 600) was used to compute the crystalline size using Scherrer's equation for two values between 20° and 80°, the crystalline structure of thin films was used to calculate the X-ray diffraction XRD technique. [15]. A UV/VIS spectrophotometer was used to assess the transmittance T and absorbance A spectrum in the wavelength range (400-1100 nm) of coated samples.

## 3. Results and discussion

#### **3.1.** Structural properties

Figure 1 depicts the XRD patterns of all thin films placed on glass at annealing temperatures of (300, 348, 398, and 448) k. The results of the samples are consistent with established standards, as evidenced by ASTM card No. 24-1041 [19], and the graph shows that the samples have an orthorhombic polycrystalline structure with  $Ag_2Se_{0.8}Te_{0.2}$  (031& 032, and 204) peaks. Table 1 shows the values for d ,(hkl), and average crystallite size (D). These findings are consistent with ASTM standards [16]. Crystallite size (D) may be calculated using Scherrer's formulation [17], although crystallite size rises as peak intensities increase owing to annealing. This implies that the system's regularity and reduced defects have improved the crystalline layers. [18]

$$D = \frac{0.94 \lambda}{(B) \cos \theta}$$
(1)

B (FWHM). is the width of the diffraction peak at half maximum intensity.

( $\theta$ ) the Bragg's angle,( $\lambda$ ) was the wavelength X-ray equal (1.54056 Å) and (FWHM) the full width half maxima of the main peak

Microstrain ( $\mathcal{E}$ ) for fabricated thin films can be calculated from the equation below:



Fig. 1. The XRD pattern for annealing temperature (300,348, 398, and 448) k,  $Ag_2Se_{0.8}Te_{0.2}$ thin films.

Table 1. X-ray Diffraction	on designation for Ag	$g_2Se_0.8Te02$ thin	film at	annealing	temperatures
	(300,348,39	98, and448) k.			

Thin films (nm)	Ta(k)	$2\theta(^{\circ}deg)$	d (A <sup>0</sup> )	Gs	DIS (lines.m <sup>-</sup>	(hkl)
Ag <sub>2</sub> Se <sub>0.8</sub> Te <sub>0.2</sub>	300	39.986	2.252	73.6043	5.8434	031
	348	39.987	2.251	78.8623	5.72048	031
	398	39.988	2.247	84.1201	5.39717	031
	448	39.989	2.245	88.3261	5.15541	031
ASTM	-	39.966	2.254	-	-	031

The AFM micrograph of  $Ag_2Se_{0.8}Te_{0.2}$  films at different temperatures (300, 348, 398, and 448) k. are depicted in Figure 3D for films with thicknesses of 350 nm. Table (2) displays the average diameter size, root mean square (Rrms), and surface roughness measurements (Rs). Surface morphology investigations support the structural and optical findings. The small islands, which operate like bubbles, may retain information. The metallic finish of the system produces reflecting mirrors and infrared reflections. The films are appropriate for data storage and optically reflecting mirrors. A slight variation in morphology by temperature will improve the use of this ternary system in heat reflection. Because of the thin film, the atoms re-spread, migrate, and grow the crystal grains along the low-stress directions, resulting in an increase in root mean square and surface roughness compared to the  $Ag_2Se_{0.8}Te_{0.2}$  beast. [19-20]

Table 2. Average Roughness, Root Mean Diameter, and Annealing Temperature for Ag2Se0.8Te0 (300, 348, 398, and 448 k.

Thin Film ( nm)	Ta(k)	Average (Diameter) (nm)	Roughness (Average) (nm)	(RMS) (nm)
Ag <sub>2</sub> Se0.8Te0.2	300	116.36	3.85	5.08
	348	161.26	3.93	5.42
	398	167.62	4.22	5.72
	448	171.02	4.31	5.88

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Fig. 2. Thin Flim Ag<sub>2</sub>Se<sub>0.8</sub>Te<sub>0.2</sub> 3D AFM pictures at annealing temperatures of (300, 348, 398, and 448) k.

## **3.2. Optical properties**

Figure 3 depicts the absorption spectra of  $Ag_2Se_{0.8}Te0.2$  thin films; absorption characteristics can be considered a valuable tool for thin film analysis. Figure (3) clearly shows that the absorption was growing abruptly and the optical transmittance of the thin films produced of  $Ag_2Se_{0.8}Te_{0.2}$ , wavelength range between 400 nm and 800 nm, and that the absorbance rose with increasing annealing temperature (300,348,398,and 448) of  $Ag_2Se_{0.8}Te_{0.2}$ . In the UV-VIS-NR area, the transmittance spectra is quite low, as shown in fig.3. When the electromagnetic spectrum is awakened, the transmittance spectra decreases (Ta) Because of the very low transmittance in the visible area,  $Ag_2Se_{0.8}Te_{0.2}$  films are required as a desirable aesthetical window glazing material. The optical transmittance spectra are used to compute the absorption coefficient, which is a function of photon energy (hu)[21-22]

$$\alpha h \upsilon = D (h \upsilon - Eg)$$
(3)

$$\alpha = 2.303 \frac{A}{t} \tag{4}$$

A = absorbance, T = thickness : absorption coefficient, hv= incident photon energy, D= is a constant that is affected by temperature as well as the parameters of the valence and conduction bands.



Fig. 3. Absorbance and transmittance of, Ag2Se0.8Te0.2 at annealing temperatures of (300, 348, 398, and 448) k thin film.



Fig.4. Shows the (hv)2 versus (hv) and refractive index of a thin film on glass substrates at various annealing temperatures (300, 348, 398, and 448)°K.

Figure 4 depicts the optical energy gap of the generated films. The energy gap was calculated using the Tauc equation. This may be accomplished by extrapolating the Tauc equation to zero absorption. Figure 4 shows the fluctuation of Eg thin films at (300, 348, 398, and 448) k. (4). The permitted direct transition optical energy gaps of films were calculated from (2&1.7&1.65and1.6) eV, which agrees well with [20–17]. This means that the energy band gaps for vacuum-annealed samples are smaller. It is reduced because of the dopant atoms at the grain boundaries, and greater absorbance may be obtained in Ag<sub>2</sub>Se<sub>0.8</sub>Te<sub>0.2</sub>. The Urbach law is used to compute the absorption coefficient. Table 1 shows the values before and after vacuum annealing in this investigation (3). These data show an increase in the number of localized states in the band gap following annealing [5]. Because of their high values, these films are a desirable material for photovoltaic applications. At 448 K, the  $Ag_2Se_{0.8}Te_{0.2}$  film exhibits the greatest values in the wavelength range (400-800 nm); this behavior may be compared to XRD and AFM data to understand the association between surface shape and rising absorbance. Samples of  $Ag_2Se_{0.8}Te_{0.2}$ show a high absorption.[25-26]. The refractive index (n) (1.65&1.4&1.6&1.25) decreased during annealing (348, 348, and 448), indicating minor dielectric loss. The best optical constants were obtained when using a vacuum annealing effect of 448 K [22–24].

Thin film (nm)	Ta(k)	Eg <sup>opt</sup> (eV)	$\alpha \times 10^4 \text{ cm}^{-1}$
	300	2	4.1
$Ag_{2}Se_{0.8}Te_{0.2}$	348	1.7	4.2
	398	1.65	4.7
	448	1.6	5.6

 Table 3. Displays the Ag2Se0.8Te0.2 absorption coefficient and direct optical energy gap for thin films annealed at different temperatures (300, 348, 398, and 448 °K).

# 4. Conclusion

In this study,  $Ag_2Se_{0.8}Te_{0.2}$  thin films were successfully deposited utilizing the thermally evaporated deposition approach, which was validated by powder XRD and utilized to produce  $Ag_2Se_{0.8}Te_{0.2}$  thin films by the thermal evaporation technique at different annealing temperatures (300, 348, 398, and 405 °K). The findings of AFM methods indicate that the grain size increases as (448 k) increases, leading to an increase in the grain boundary, whereas the  $Ag_2Se_{0.8}Te_{0.2}$  value ranges from (116.36&161.26&167.62 and 171.02 nm). At various annealing temperatures, the band gap was found to have indirectly risen from (2, 1.7, 1,65, and 1.6) eV The films were shown to have a high UV absorbance and to underestimate it as the wavelength rose. Furthermore, their transmittance is usually exaggerated. demonstrate the benefits of the thin film for aesthetic window glazing and the formation of photovoltaic p-n junctions. cell .

## References

[1] C. Vijayan, M. Pandiaraman, N. Soundararajan, R.Chandramohan, V. Dhanasekeran, K. Sundaram, T. Mahalingam and A. John Peter:J. Mater. Sci. Mater. Electron, 22, 545,2010; https://doi.org/10.1007/s10854-010-0175-y

[2] C. Vijayan, N. Soundararajan, R.Chandramohan, V. Dhanasekeran, K. Sundaram, K. Neivasagam and T. Mahalingam: J. Microsc., 243, 261, 2011;

https://doi.org/10.1111/j.1365-2818.2011.03500.x

[3] Ruizhi, C., Dongsheng, X., Guolin, G. & Linlin, G., Electrochem. Commun. 5, 579-583, 2003; https://doi.org/10.1016/S1388-2481(03)00133-4

[4] Das, V.D. & Karunakaran, D., Phys. Rev. B 39, 10872-10878, 1989; https://doi.org/10.1103/PhysRevB.39.10872

[5] Ferhat, M. & Nagao, J., J. Appl. Phys. 88, 813-820, 2000; https://doi.org/10.1063/1.373741

[6] Xu, R., Husmann, A., Rosenbaum, T.F., Saboungi, M.L., Enderby, J.E. & Littlewood, P.B., Nature 390, 57-60, 1997; <u>https://doi.org/10.1038/36306</u>

[7] Glanville, Y.J., Narehood, D.G., Sokol, P.E., Amma, A.& Mallouk, T., J. Mater. Chem. 12, 433-2434, 2002; <u>https://doi.org/10.1039/b202913h</u>

[8] Khan, S.A., Zulfequar, M. & Husain, M., Vacuum, 72, 291-296, 2003; https://doi.org/10.1016/j.vacuum.2003.08.006

[9] Ruizhi, C., Dongsheng, X., Guolin, G. & Linlin, G., Electrochem. Commun. 5, (2003),579-583; <u>https://doi.org/10.1016/S1388-2481(03)00133-4</u>

[10] Xue, M.Z., Chong, S.C., Yao, J. & Fu, Z.W., Electrochim. Acta 51, 3287-3291, 2006; https://doi.org/10.1016/j.electacta.2005.09.020

[11] V. M. Dzhagan, M. Ya Valakh, A. E. Raevskaya, A. L. Stroyuk, S. Ya Kuchmiy and D. R. T. Zahn: Nanotechnology, 19,305707, 2008; <u>https://doi.org/10.1088/0957-4484/19/30/305707</u>

[12] B. K. H. Al-Maiyaly, B. H. Hussein, H. K. Hassun, Journal of Ovonic Research, 16 (5), 267 - 271 (2021).

[13] P. Sharma, V. Sharma, S.C. Katyal, Chalcogen. Lett. 3(10), 73,(2006)

[14] H. Liu, B. Zhang, H. Shi, Y. Tang, K. Jiao, and X. Fu, J. Mater. Chem. 18, 2573 (2008); https://doi.org/10.1039/b719207j

[15] V. S. Vinogradov, G. Karczewski, I. V. Kucherenko, N. N. Mel'nik and P. Fernandez: Phys. Solid State, 50(1), 164, 2008; <u>https://doi.org/10.1134/S1063783408010290</u>

[16] JCPDS, "International Center for Diffraction Data," ASTM data files card No. 24-1041, 1972
[17] Hiba M. Ali , I. H. Khudayer, Journal of Ovonic Research, Vol. 18, No. 5, september - October 2022; <u>https://doi.org/10.15251/JOR.2022.185.675</u>

[18] M. G. Sridharan, M. Mekaladevi, S. K. Narayandass, D. Mangalaraj and H. Chul Lee: J. Optoelectron. Adv. M. 7(3), 1479 (2005).

[19] Vijayan, C., Pandiaraman, M., Soundararajan, N., Chandramohan, R., Dhanasekaran, V., Sundaram, K., Mahalingam, T. & John Peter, A., J. Mater. Sci. Mater. Electron(2010), 22, 545-550; <u>https://doi.org/10.1007/s10854-010-0175-y</u>

[20] Hiba M. Ali, Hanan K. Hassun , Bushra. K.H.al-Maiyaly, Auday H. Shaban, Energy Procedia,(157) 90 99 2019; <u>https://doi.org/10.1016/j.egypro.2018.11.168</u>

[21] Suha. A. Fadaam , Hiba M. Ali, Ayad.Ahmed.Salih, Maithm.A.Obaid, Ali Sabeeh Ali and Nadir F.Habubi, Journal of Physics: Conference Series, 2nd International Conference on Physics and Applied Sciences (ICPAS 2021), 196301200.

[22] Hiba M Ali , Sameer A Makki, Ahmed N Abd, IOP Conf. Series: Journal of Physics: Conf. Series 1003 012073, (2018); <u>https://doi.org/10.1088/1742-6596/1003/1/012073</u>

[23] Khudayer, I. H.; and Hussien, B.H.; Study of Some Structural and Optical Properties of AgAlSe2 Thin Films, Ibn Al-Haitham J. for Pure & Appl. Sci., , 29 ( 2), 2016.

[24] Bushra,K. H.;Characterization of n-CdO:Mg /p-Si, J. for Pure & Appl. Sci. 29 (3),14-25,2016.

[25] C. Vijayan, M. Pandiaraman, N. Soundararajan, Mater Sci: Mater Electron 22,545-550, 2011; https://doi.org/10.1007/s10854-010-0175-y

[26]Bushra H. Hussein, Iman Hameed Khudayer, Mohammed Hamid Mustafa, Auday H. Shaban, An International Journal (PIE) 13(2), 173 (2019); https://doi.org/10.1504/PIE.2019.099358