

Study structure and optical properties of Ag_2Se , $\text{Ag}_2\text{Se}_{0.8}\text{Te}_{0.2}$ and $\text{Ag}_2\text{Se}_{0.8}\text{S}_{0.2}$ thin films

Hiba M. Ali*, I. H. Khudayer

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

Silver sulfide and the thin films $\text{Ag}_2\text{Se}_{0.8}\text{Te}_{0.2}$ and $\text{Ag}_2\text{Se}_{0.8}\text{S}_{0.2}$ created by the thermal evaporation process on glass with a thickness of 350 nm were examined for their structural and optical properties. These films were made at a temperature of 300 K. According to the X-ray diffraction investigation, the films are polycrystalline and have an initial orthorhombic phase. Using X-ray diffraction research, the crystallization orientations of Ag_2Se and $\text{Ag}_2\text{Se}_{0.8}\text{Te}_{0.2}$ & $\text{Ag}_2\text{Se}_{0.8}\text{S}_{0.2}$ (23.304, 49.91) were discovered (XRD). As (Ag_2Se and $\text{Ag}_2\text{Se}_{0.8}\text{Te}_{0.2}$ & $\text{Ag}_2\text{Se}_{0.8}\text{S}_{0.2}$) absorption coefficient fell from (470-774) nm, the optical band gap increased (2.15 & 2 & 2.25eV). For instance, the characteristics of thin films made of $\text{Ag}_2\text{Se}_{0.8}\text{Te}_{0.2}$ and $\text{Ag}_2\text{Se}_{0.8}\text{S}_{0.2}$ and silver sulfide have been studied.

(Received July 30, 2022; Accepted October 12, 2022)

Keywords: Characterization of the structure, Optical properties, Ag_2Se thin film

1. Introduction

Researchers are interested in silver selenide because of its use in switching devices. Because electron transport is limited in at least one direction, semiconducting materials exhibit distinctive structural and visual features. Semiconductors' size-dependent structural, optical, and electrical properties play an essential role in science and technology. In the fields of optics and electronics, phase-changing chalcogenide materials offer a wide range of applications [1-3]. Essential materials for Schottky barriers, solar cells, and electronic engineering are binary and ternary semiconductors. Furthermore, silver selenide is a member of the superionic conductor family, which is of current and future technological relevance. The thickness dependence of the transition temperature and activation energy was studied. The low-temperature phase, α - Ag_2Se , has an orthorhombic structure, while the high-temperature phase β - Ag_2Se , has a bcc structure. With a transition temperature of roughly 408 K or 395 K, silver selenide exists as a high-temperature cubic phase (α), a low-temperature orthorhombic (β), and a tetragonal phase. Furthermore, the shift from b to a occurs via an intermediate phase; the duration of this new phase rises from cycle to cycle, and structural evidence available in the literature contradicts the low-temperature phase[4]. Various publications have described the material as tetragonal, orthorhombic, and monoclinic.

Silver selenide thin films have been prepared using a variety of techniques. Vacuum evaporation of a silver selenide alloy was used by to create the films[2]. Using the explosive evaporation of the powdered substance in vacuum on various surfaces, [4] reported on the chemical bath deposition approach [5–6]. films were created by flash evaporation in [7] reported on employing chemicals to convert silver films into silver selenide films [8] used a method of vacuum deposition of selenium on to glass substrates temperature. [9-10] Ag_2Se crystals were produced by the reaction of selenium films with silver films at room temperature .examined the characteristics of thin films produced by the successive evaporation of components (Ag first, then Se) in a vacuum of around 10^6 Torr [11] The films show metallic behaviour between 77 K and 300

*Corresponding author: hibaomer79@gmail.com
<https://doi.org/10.15251/JOR.2022.185.675>

K and with a chemical composition, $\text{Ag}_{2-x}\text{Se}_1+x$ with $0.01 \leq x \leq 0.05$ [12] have developed an alloy to fabricate highly ordered Ag_2Se arrays by thermal evaporation prepared $\text{Ag}_2\text{Se}_{1-x}\text{Te}_x$ and

$\text{Ag}_2\text{Se}_{1-x}\text{S}_x$ thermal evaporation has been used to create crystalline $\text{b-Ag}_2\text{Se}$ in a variety of forms. In this situation, we tried a technique with little prior research. Here, we describe the thermal evaporation process used to generate an Ag_2Se thin film as well as its structural and optical characteristics [13-14]

2. Experimental

The alloy was utilized to create thin films of Ag_2Se , which were formed on glass substrates using the thermal evaporation method in a high vacuum system and have a thickness of roughly 350 nm on one type of substrate (glass slides). [15] Using the molybdenum boat's (Edwards-Unit 306) system, thermal evaporation procedures were used to prepare the thin films that were created. The glass slides were divided into pieces measuring (1.5×1.5) cm in accordance with the removal of the base holder by the use of a steel blade. To get rid of the stain and the protein substance on the glass slides, they were washed using an easy-to-use chemical detergent solution. When an X-ray diffractometer (SHIMADZU Japan XRD 600) has been 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. [16]. The transmittance T and the absorbance A spectrum in the wavelength range (400–1100 nm) of coated samples' optical properties was evaluated using a UV/VIS spectrophotometer, and the energy gap was computed using the Tauc equation [17-18].

3. Results and discussion

3.1. Structural Properties

The figure (1) shows the XRD patterns of all thin films that were deposited on glass at a temperature of 300 k. According to the graph, the samples exhibit an orthorhombic polycrystalline structure that contains Ag_2Se and $\text{Ag}_2\text{Se}_{0.8}\text{Te}_{0.2}$ (031), (032), (042) & (204) peaks, and their results are in compliance with established standards, as shown by ASTM card No. 24-1041 [19]. Table 1 displays the values for the lattice constant (a), d (hkl), and average crystallite size (D). These results are in good settlement with [5]. The crystallite size (D) can calculate with Scherrer's formulation [20]

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

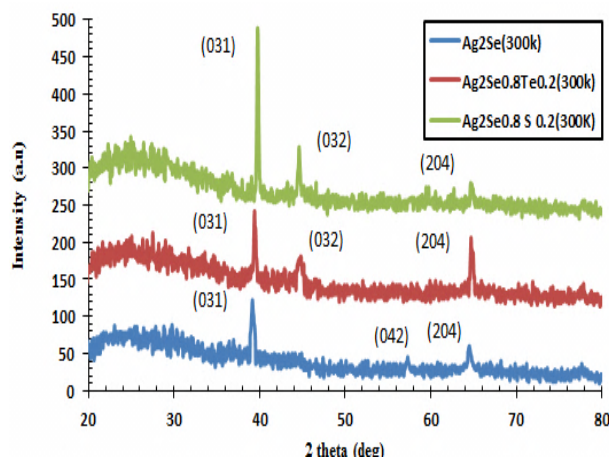


Fig. 1. The XRD pattern of Ag_2Se , $\text{Ag}_2\text{Se}_{0.8}\text{Te}_{0.2}$ and $\text{Ag}_2\text{Se}_{0.8}\text{S}_{0.2}$ thin film.S

Table 1. X-ray Diffraction assignment Ag_2Se , $Ag_2Se_{0.8}Te_{0.2}$ and $Ag_2Se_{0.8}S_{0.2}$ thin film. S.

Thin films	$2\theta(^{\circ})$	$d(A^{\circ})$	G_s	DIS (lines.m ⁻²)	(hkl)
Ag_2Se	39.15	2.28	70.47	2.01	031
$Ag_2Se_{0.8}Te_{0.2}$	39.48	1.60	73.48	1.85	031
$Ag_2Se_{0.8}S_{0.2}$	39.87	2.25	45.51	4.82	031
ASTM	39.99	2.25	-	-	031

AFM experiments were carried out on the Ag_2Se , $Ag_2Se_{0.8}Te_{0.2}$, and $Ag_2Se_{0.8}S_{0.2}$ films depicted in figure (2). Table (2) shows the values for the average diameter size, root mean square (Rrms), and surface roughness (Rs). The findings revealed that grains are compactly combined to form ridges and clusters along the surface of Ag_2Se , $Ag_2Se_{0.8}Te_{0.2}$, and $Ag_2Se_{0.8}S_{0.2}$ films. 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 due to thin film. Increases in Ag_2Se , $Ag_2Se_{0.8}Te_{0.2}$, and $Ag_2Se_{0.8}S_{0.2}$ decrease cause recrystallization in grains .than the best [24]

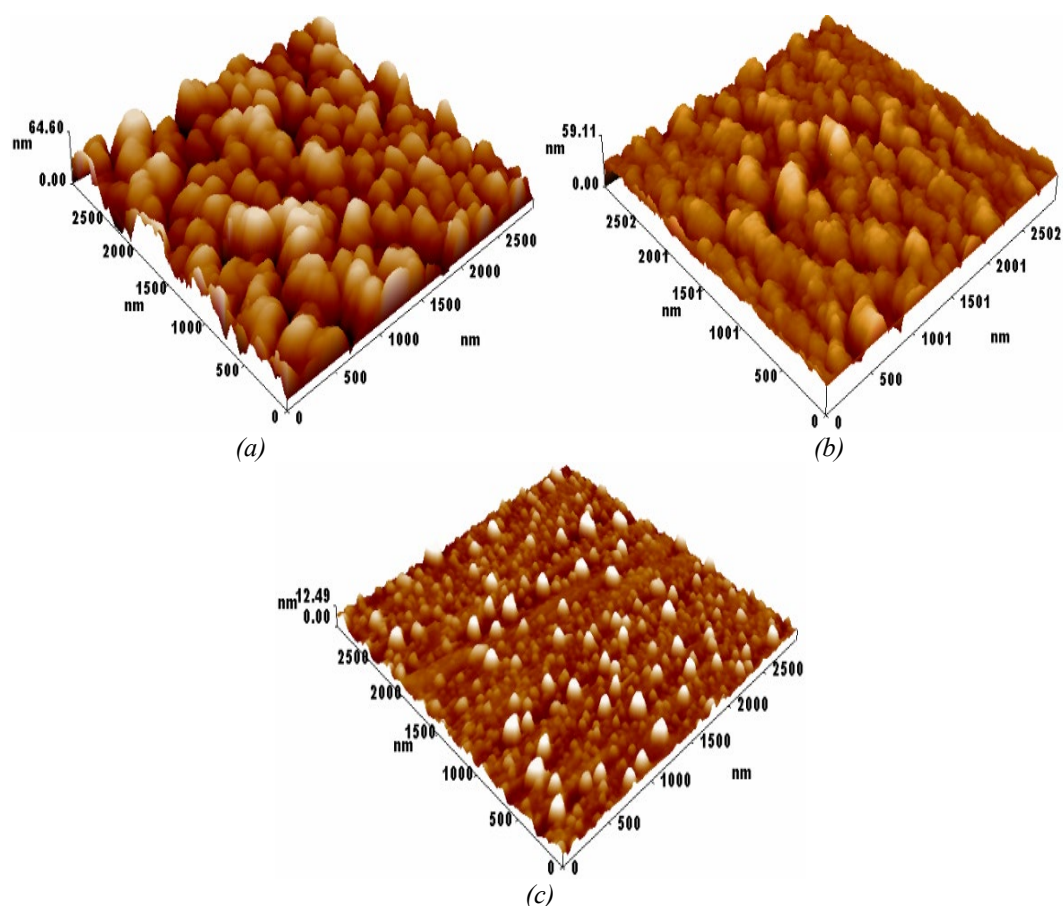


Fig. 2. 3D AFM images of Thin Flim (a) Ag_2Se , (b) $Ag_2Se_{0.8}Te_{0.2}$ (c) $Ag_2Se_{0.8}S_{0.2}$ at (300k).

Table 2. Root Mean ,Average Diameter, RoughnessAverage (a) Ag_2Se , (b) $Ag_2Se_{0.8}Te_{0.2}$ (c) $Ag_2Se_{0.8}S_{0.2}$ at (300k).

Thin Film (nm) (300K)	Average (Diameter) (nm)	Roughness (Average) (nm)	(RMS) (nm)
Ag_2Se	75.74	8.16	10.2
$Ag_2Se_{0.8}Te_{0.2}$	116.36	3.93	5.08
$Ag_2Se_{0.8}S_{0.2}$	35.55	1.35	1.8

3.2. Optical Properties

Figure 3 shows the absorbance spectra and optical transmittance of the thin films made of Ag_2Se , $Ag_2Se_{0.8}Te_{0.2}$, and $Ag_2Se_{0.8}S_{0.2}$. In the wavelength range between 400 nm and 700 nm, it has been observed that the absorbance has decreased with increasing ratios of $Ag_2Se_{0.8}Te_{0.2}$ and $Ag_2Se_{0.8}S_{0.2}$. This might be due to the assistance of (Te, S) ions in the Ag_2Se lattice and improved crystallinity as a result of a decrease in crystallite size. For all samples, the transmittance rises as ratios fall; this could be a result of enhanced absorption, which could be related to the deformation of Ag_2Se brought on by (Te, S) ions. The low crystallite size values (70,74,45) nm for these films, as shown in Table 1, may account for the transmittance (10% to 22%) found for Te, S (0.2%) percent films. The best membrane in terms of crystal size is tellurium in terms of properties.

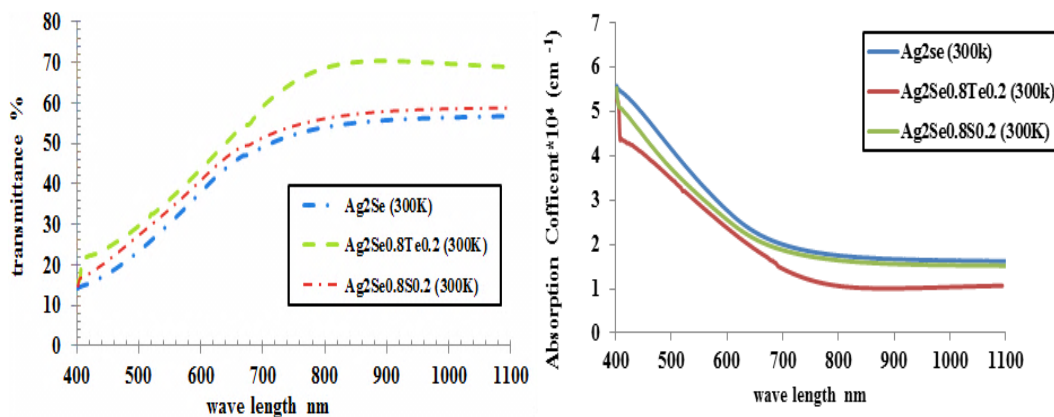


Fig. 3. Optical transmittance and absorbance of Ag_2Se , $Ag_2Se_{0.8}Te_{0.2}$ and $Ag_2Se_{0.8}S_{0.2}$ thin film.

Figure 4 shows the produced films' optical energy gap. The Tauc equation was used to determine the optical energy gap in the high absorption region [21,22]. For Ag_2Se , $Ag_2Se_{0.8}Te_{0.2}$, and $Ag_2Se_{0.8}S_{0.2}$ thin films, the energy band-gap values were 2.15, 2, and 2.25, respectively, as shown in Table 3. The density of localized states in the E_g increases due to the observed decreasing energy-gap values caused by an increase in film defects. optical energy gap movement in the vicinity of more extended wavelength red. The value corresponds to [5]. Ag_2Se , $Ag_2Se_{0.8}Te_{0.2}$, and $Ag_2Se_{0.8}S_{0.2}$ samples have high absorbance, making them suitable as an optical material for solar-cell applications. [23].

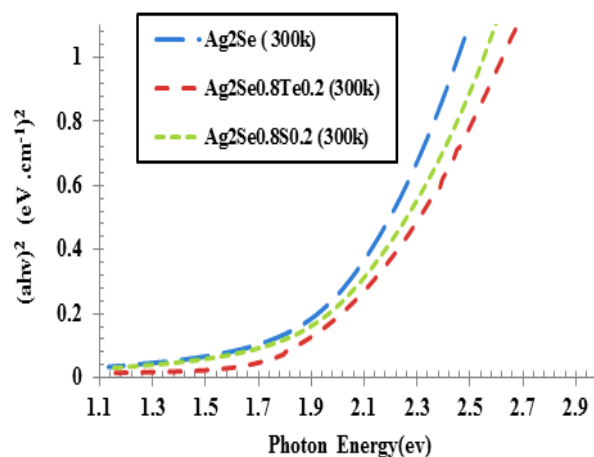


Fig. 4 The $(\alpha hv)^2$ versus (hv) Ag_2Se , $Ag_2Se_{0.8}Te_{0.2}$ and $Ag_2Se_{0.8}S_{0.2}$ thin film on glass substrates.

Table 3. Direct optical Energy gap and absorption coefficient for Ag_2Se , $Ag_2Se_{0.8}Te_{0.2}$ and $Ag_2Se_{0.8}S_{0.2}$ thin film.

$\lambda=400\text{nm}$		
Sample	E_g^{opt} (eV)	$\alpha \times 10^4 \text{ cm}^{-1}$
Ag_2Se	2.15	5.53
$Ag_2Se_{0.8}Te_{0.2}$	2	5.10
$Ag_2Se_{0.8}S_{0.2}$	2.25	5.20

4. Conclusion

The thin films of Ag_2Se , $Ag_2Se_{0.8}Te_{0.2}$, and $Ag_2Se_{0.8}S_{0.2}$ were prepared using the thermal evaporation method. Resulting from (Te, S), Ag_2Se thin films' structural and optical properties were taken into account by adding a percentage of it (0.2) and changing a percentage of Se (0.8). The XRD patterns revealed that every deposit had an orthorhombic structure and was polycrystalline. With Ag_2Se , $Ag_2Se_{0.8}Te_{0.2}$, and $Ag_2Se_{0.8}S_{0.2}$ thin films, the crystallite size value from (70, 74, 45) nm Ag_2Se , $Ag_2Se_{0.8}Te_{0.2}$, and $Ag_2Se_{0.8}S_{0.2}$ cause increased atomic volume. AFM techniques results display that the decrease in grain size when (300k) increase which lead to increase the grain boundary but $Ag_2Se_{0.8}Te_{0.2}$ increase of grain size but the $Ag_2Se_{0.8}S_{0.2}$ decreased the grain size. The optical band-gap of films increased from (2.15, 2, 2.25) eV due to their good crystallite size, improved absorption coefficient, and other factors. Ag_2Se , $Ag_2Se_{0.8}Te_{0.2}$, and $Ag_2Se_{0.8}S_{0.2}$ samples have high absorbance, making them suitable as an optical material for solar-cell applications.

References

- [1] N. Yamada, Mater Res Soc Bull 21, 48, 1996; <https://doi.org/10.1557/S0883769400036368>
- [2] Damodara Das V and Karunakaran J. Appl. Phys. 67 878, 1990; <https://doi.org/10.1063/1.345747>
- [3] Okabe Toshio and Ura Katsuhiko J. Appl. Cryst. 27 140, 1994; <https://doi.org/10.1107/S0021889893009094>
- [4] Abdullayev A G, Shafizade R B, Krupnikov E S and Kiriluk K V 1983 Thin Solid Films 106;

[https://doi.org/10.1016/0040-6090\(83\)90479-0](https://doi.org/10.1016/0040-6090(83)90479-0)

[5] Somogyi K and Safran G 1995 J. Appl. Phys. 78 6855; <https://doi.org/10.1063/1.360449>

[6] Somogyi K and Safran G 1995 Vacuum 46 1055; [https://doi.org/10.1016/0042-207X\(95\)00105-0](https://doi.org/10.1016/0042-207X(95)00105-0)

[7] Okabe T and Ura K 1994 J. Appl. Crystallogr. 27 140;

<https://doi.org/10.1107/S0021889893009094>

[8] Sharma K C, Sharma R P and Garg J C 1990 Indian J. Pure Appl. Phys. 28 546

[9] Bernede J C, Conan A, Fouesnant E, El Bouchairi B and Goureaux G Thin Solid Films 97 165, 1982; [https://doi.org/10.1016/0040-6090\(82\)90225-5](https://doi.org/10.1016/0040-6090(82)90225-5)

[10] Constantinescu L V 1976 Thin Solid Films 32 333; [https://doi.org/10.1016/0040-6090\(76\)90325-4](https://doi.org/10.1016/0040-6090(76)90325-4)

[11] Saito Y, Sato M and Shijori M 1981 Thin Solid Films 79 257; [https://doi.org/10.1016/0040-6090\(81\)90314-X](https://doi.org/10.1016/0040-6090(81)90314-X)

[12] M C Santhosh Kumar and B Pradeep, Institute of Physics Publishing, Semicond. Sci. Technol. 17, 261-265, (2002); <https://doi.org/10.1088/0268-1242/17/3/314>

[13] Y. Cui, G. Chen, J. Ren, M. Shao, Y. Xie, Y. Qian, J. Sol. Stat.Chem. 172, 17 (2003); [https://doi.org/10.1016/S0022-4596\(02\)00040-3](https://doi.org/10.1016/S0022-4596(02)00040-3)

[14] M.-Z. Xue, S.-C. Cheng, J. Yao, Z.-W. Fu, Electrochim. Acta 51,3287 (2006); <https://doi.org/10.1016/j.electacta.2005.09.020>

[15] Hiba M. Ali, Hanan K. Hassun , Bushra. K.H.al-Maiyaly, Auday H. Shaban, Technologies and Materials for Renewable Energy, Environment and Sustainability - Tmrees18, Energy Procedia,(157) 90 99 2019; <https://doi.org/10.1016/j.egypro.2018.11.168>

[16] Suha. A. Fadaam1 , Hiba M. Ali, Ayad.Ahmed.Salih, Maithm.A.Obaid3, AliSabeeh Ali and Nadir F.Habubi, Journal of Physics: Conference Series, 2nd International Conference on Physics and Applied Sciences (ICPAS 2021), 1963012003

[17] Suha Fadaam, Hiba Ali, Auday Shaban and Saja Ahmed, AIP Conference Proceeding, 1551-7616,2020.

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

[19] JCPDS, "International Center for Diffraction Data," ASTM data files card No. 24-1041, 1972

[20] Hanan Kadhem Hassun "Study of Photodetector Properties ZnTe:Al/Si prepared by Thermal Evaporation" Ph.D. thesis, University of Baghdad, college of Education for pure science Ibn Alhaitham, (2017).

[21] B. K. H. AL-Maiyal, B. H. Hussein and H. K. Hassun, Journal of Ovonic Research, 16 (5), (2020).

[22] C. Vijayan • M. Pandiaraman • N. Soundararajan, Mater Sci: Mater Electron22:545-550, (2011); <https://doi.org/10.1007/s10854-010-0175-y>

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

[24] C. Vijayan, N. Soundararajan,R.Chandramohan,V. Dhanasekaran, Journal of Microscopy, Vol. 243, Pt 3 2011, pp. 267-272;

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