

ORIGINAL RESEARCH ARTICLE

Synthesis and Characterization of Quaternary Copper Barium Iron Sulphide Thin Films by Chemical Bath Deposition

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ABSTRACT

Copper barium iron sulphide (CBFS) thin films were synthesized using a chemical bath deposition (CBD) method on glass substrates for 10 hours. The study used solutions of copper (II) chloride dehydrate, barium chloride, iron (II) chloride, and thiourea as the sources of the elements (copper, barium, iron and sulphur) to fabricate films of thickness 105.81 nm at a pH of 9.60. Fourier Transform Infrared (FTIR) Spectroscopy was employed to analyze the chemical characteristics of the aqueous precursor and the deposited films at 30 °C. Experimental observations revealed distinctive CBFS absorption bands below 900 cm⁻¹ in the FTIR spectrum of the precursor. The optical band gap energy was determined to be 1.36 ± 0.05 eV, with the absorbance decreasing (from 0.6 to 0.3 au) as the wavelength increased from 300 to 1000 nm. The optical constants of extinction coefficient and optical conductivity were found to be 0.05 and 0.7 S⁻¹ respectively at 3.50 eV. Scanning electron microscopy (SEM) micrographs showed that the films were crack-free, rough, and uniformly covered with grains of various shapes. Electron dispersive x-ray (EDX) revealed that the deposited material consists of copper, barium, iron and sulphur. X-ray diffraction (XRD) analysis confirmed the crystalline structure of the deposited films. Hence, the crystalline sizes (D), dislocation density (δ), and the strain function (ε) were also evaluated to range from 29.91 to 135.53 nm, 0.54 × 10¹⁴ to 11.2 × 10¹⁴, and 0.00079 to 0.00473, respectively. These findings suggest that the synthesized CBFS thin films have potential for integration in diverse electronic applications.

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INTRODUCTION

A wide range of materials have been fabricated as thin films due to their promising technical and scientific applications. These films have an extensive variety of uses, from microelectronic components to large-area coatings for windows (Emegha et al., 2022; Shepelin et al., 2023; Adebisi et al., 2025). Thin films can be conceptualized as the near-surface region of a material, with thicknesses ranging from fractions of a nanometer to several micrometers (Arun et al., 2025). These thin films exhibit properties that are markedly different from those of the bulk materials they are composed of (Arun et al., 2025; Abdullahi et al., 2025; Etim et al., 2025; Ibrahim et al., 2025; Yahaya et al., 2022) as their characteristics are dependent on a multitude of interrelated parameters as well as the specific fabrication method employed (Shepelin et al., 2023). The interface between thin films and their underlying substrates can significantly impact the internal physical attributes and behaviors of the material.

This reciprocal interaction may give rise to entirely novel phenomena (Sarf et al., 2024; Arun et al., 2025).

The fabrication of thin film materials has been a crucial driver in the development of innovative electrical devices, particularly high-efficiency solar cells (Palazon, 2022; Emegha and Nwanze, 2022; Llorens Balada, 2024). Quaternary metal sulphide semiconductors have become a central focus in photovoltaic technologies due to their diverse and versatile properties (Turnley and Agrawal, 2024). The photovoltaic (PV) market is continuously expanding, employing novel materials and modifying conventional manufacturing processes (Turnley and Agrawal, 2024). In recent years, Cu(InGa)Se₂ (CIGS) and CuIn(S,Se) (CIS) have been established as excellent materials for energy conversion devices. For instance, CIGS-based thin film solar cells have shown record energy conversion efficiencies greater than 20% (Efe et al., 2019). However, such CIGS-based

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devices contain rare and expensive materials (In and Ga). This could make such devices expensive and beyond human reach. Consequently, there is a need to develop materials that are cheap and abundant in nature, which can be deposited by methods that ensure simplicity, leading to high efficiencies in device performance (Efe et al., 2019; Emegha et al., 2022). Materials such as $\text{Cu}_2\text{ZnSnS}_4$ (CZTS), $\text{Cu}_2\text{FeSnS}_4$ (CFTS), $\text{Cu}_2\text{BaSnS}_4$ (CBTS), CuBaFeS_4 , and $\text{Cu}_2\text{BaSn(S,Se)}_4$ are promising materials that can replace CIGS in energy conversion devices. Among these materials, Copper–Barium–Iron Sulphide (Cu–Ba–Fe–S or CBFS) remains one of the least explored quaternary sulphides. Thus, replacing Sn or Fe with Ba introduces significant modifications to crystal chemistry, electronic structure, defect formation, grain growth, and optical behavior (Okafor et al., 2025). Despite its promising characteristics, systematic studies on CZBS remain extremely limited, leaving many of its physical properties unknown.

In this work, we fabricated copper barium iron sulphide (CBFS) thin films using the CBD technique. The flexibility of the CBD method has led to its selection as the primary deposition approach for the production of thin films and coatings for various applications (Elete et al., 2023; Zhu et al., 2025). The interest in CBFS stems from the potential to engineer the compound parameters during deposition. Furthermore, CBFS compounds are garnering increasing attention due to their favorable performance characteristics, moderately simple chemistry, and the lack of significant environmental concerns associated with their use (Emegha et al., 2022). This study presents for the first time the fabrication and analysis of the quaternary CBFS thin films through the CBD technique.

THE EXPERIMENTAL PROCEDURE

2.1 Materials and Chemicals

The copper barium iron sulphide thin films were synthesized via the CBD process using copper (II) chloride dehydrate ($\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$), barium chloride (BaCl_2), iron (II) chloride (FeCl_2), thiourea [$\text{SC}(\text{NH}_2)_2$], ammonia solution (NH_4OH), and ethylenediaminetetraacetic acid (EDTA). The chemicals were all analytical-grade and used without further purification.

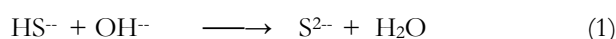
2.2 Substrate Cleaning Procedure

Soda-lime glass slides of various sizes were utilized as the substrates for the film deposition. Prior to the deposition process, the substrates were dipped in a concentrated 1.0 M hydrochloric acid (HCl) solution for 24 hours to eliminate any dirt or grease that might hinder the nucleation of the films. Then, the substrates were gently cleaned with liquid detergent and cotton wool to further remove any remaining dirt, rinsed in distilled water, and allowed to air dry at room temperature.

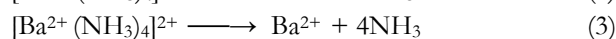
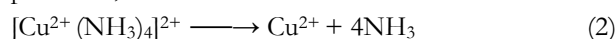
2.3 Fabrication of CBFS Thin Films

In this study, 0.5 M $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ (10 ml), 0.5 M of BaCl_2 (10 ml), 0.4 M of FeCl_2 (10 ml), and 0.2 M of $\text{SC}(\text{NH}_2)_2$ (25 mL) were dissolved separately in a 50 mL water beaker. The solutions were then mixed in the ratio of 2:1:1:2, and stirred for 30 minutes to form the CBFS precursor. Complexing agent (EDTA) was employed to slow down the formative reactions, and an ammonia solution was used to stabilize the pH of the bath at 9.60. The resulting solution was further stirred for 50 minutes at room temperature to produce a uniform solution using a magnetic stirrer. Subsequently, the clean glass substrates were immersed in the chemical solution as shown in Figure 1. The reaction was allowed to proceed for 10 hours. Finally, the substrates were washed and dried at room temperature. These preparation steps were consistently applied to maintain reproducibility across all experiments.

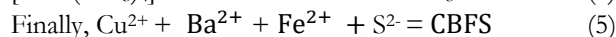
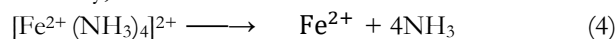
The deposition process of the material via CBD is based on the slow release of the ions by the corresponding complexing agents (EDTA Disodium salt), and subsequently the nucleation of films on the substrates. The chemical mechanism of the film formation and deposition is as follows: The decomposition of thiourea in alkaline solution (Fekadu, 2015):



When ammonia is added to the various salts solutions (Cu^{2+} , Ba^{2+} and Fe^{2+}) tetra-amine complexes are produced; thus:



Similarly,



When reactions (1), (2), (3) and (4) are adequately slow, a heterogeneous nucleation of the material would occur on the inner walls of the beakers as well as on the immersed substrates, and the deposition of the material thin films can be expected in each reaction.

2.4 Characterization of CBFS Thin Films

Fourier transform infrared spectroscopy was conducted on the precursor and film samples using a Shimadzu 8400 FTIR Spectrometer. Optical measurements of the films were performed at room temperature using a UV-vis Spectrophotometer, spanning the wavelength range of 300–1100 nm. The bandgap energy was subsequently determined from the optical data. Scanning electron microscopy incorporated with Electron dispersive x-ray (EDX) analyzer was employed to study the morphological structures of the deposited films at 1000 V, while X-ray diffraction analysis was carried out using a Bruker XRD

D8-Shimadzu system with Cu-K α radiation. The thickness of the film was measured using the weight difference method using the relations: $t = \frac{M}{2AD}$, and $M = m_a - m_b$. Here m_a is the mass of the substrates before deposition, and m_b is the mass of the substrates after deposition. A is the area of the deposited surface and D is the density of the material. The measurement was taken multiply times, and the thickness was found to be 105.81 nm.

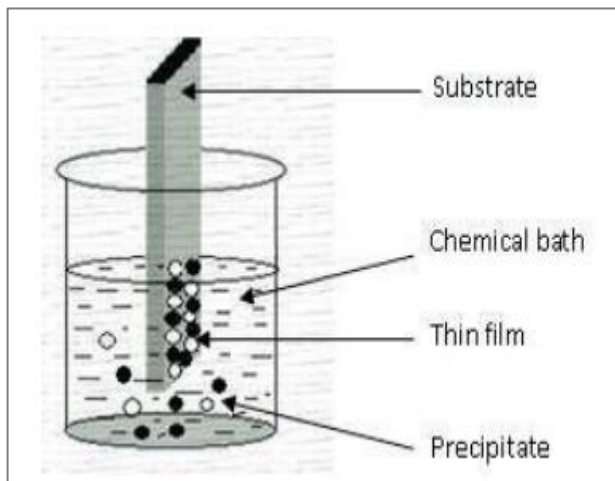


Figure 1: Chemical setup for CBFS thin film deposition (Okafor et al., 2025)

RESULTS AND DISCUSSION

The infrared spectra of the precursor and the deposited films are depicted in Figures 2 and 3. Figure 2 illustrates

the various functional groups present in the precursors. The measurement was conducted within the wavenumber range of 4000 to 500 cm^{-1} using a KBr background. The major bands are the O-H group, which was observed with three peaks at 3506.70, 3414.12 and 3342.75 cm^{-1} respectively (Efe et al., 2026). The existence of a broad OH group with multiple peaks had been reported in the literature and was due to the presence of the amino salt within the spectrum. The bands observed in the range of 2916.47 to 2033.19 cm^{-1} are attributed to the weak stretching vibrations of C-H or C-C bonds (Emegha et al., 2021). The bands at 1670.86 and 1637.62 cm^{-1} correspond to the stretching modes of C=O vibrations. The bands at 1508.38 and 1369.50 cm^{-1} are associated with the stretching vibrations of C-H bonds. The spectrum also showed a C-O vibration in the 1178.55 to 991.44 cm^{-1} region, which may be assigned to the C-H stretching. The CBFS absorption peaks were found to be below the 900 cm^{-1} bands. Similar studies have indicated that the bands of metal sulphides and oxides are always below the 900 cm^{-1} mark (Alam et al., 2022)

Figure 3 displays the deposited infrared spectra of CBFS thin films. When the signals were compared to those in Figure 2, it was evident that the distinctive bands linked to the chemical precursors were absent. The precursor underwent complete decomposition, resulting in the formation of copper barium iron sulfide thin films. This finding is consistent with the reported breakdown behavior of metal sulfides in the literature (Emegha et al., 2021).

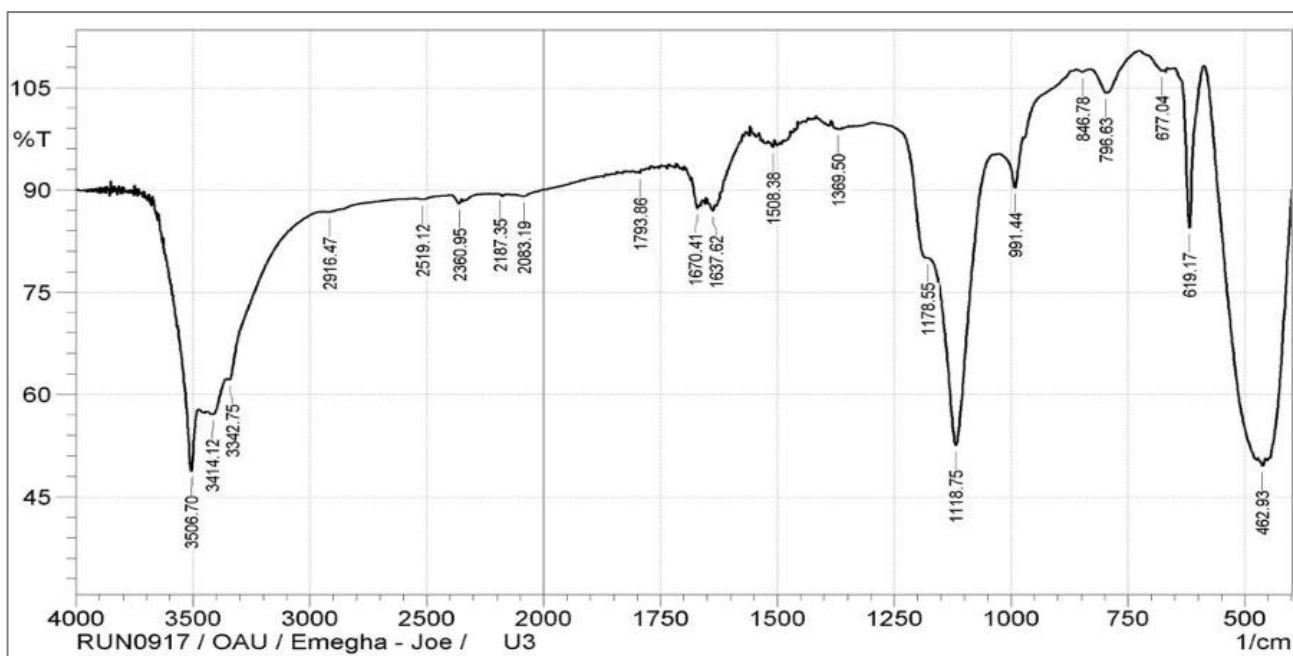


Figure 2: Infrared Spectroscopic Characteristics of CBFS Precursor

The optical characteristics of the deposited thin film materials were assessed using a UV-Vis spectrophotometer. As depicted in Figure 4, the absorption spectrum of the CBFS thin films exhibits elevated absorbance in the ultraviolet wavelength region, which gradually decreases as the wavelength increases.

The high absorbance in the ultraviolet region may be attributed to the light scattering effects arising from the nano-sized grains of the films due to variations in the spectral range (Emegha et al., 2021). Additionally, the relatively enhanced absorbance in the ultraviolet region could be associated with the presence of defects within the

CBFS thin films (Emegha et al., 2021). Correspondingly, the enhanced absorption observed in this region makes

the film a possible window material for solar cell applications (Babalola et al., 2024).

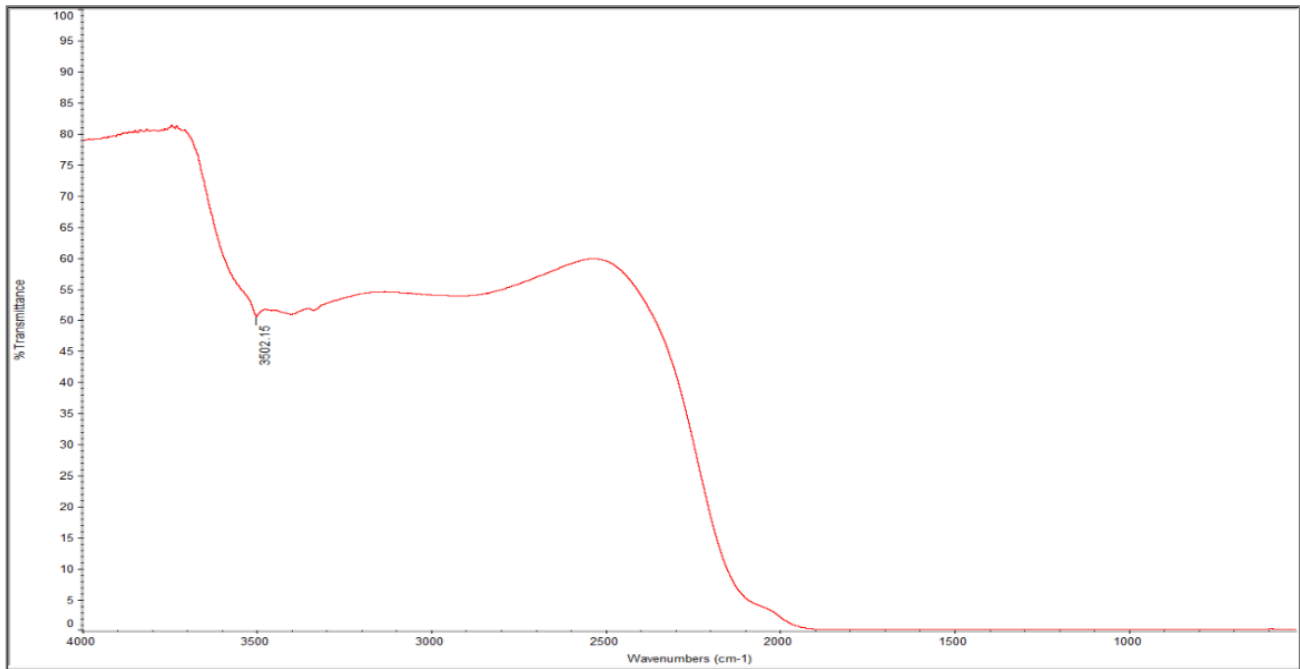


Figure 3: Infrared Spectroscopic Characteristics of CBFS thin films

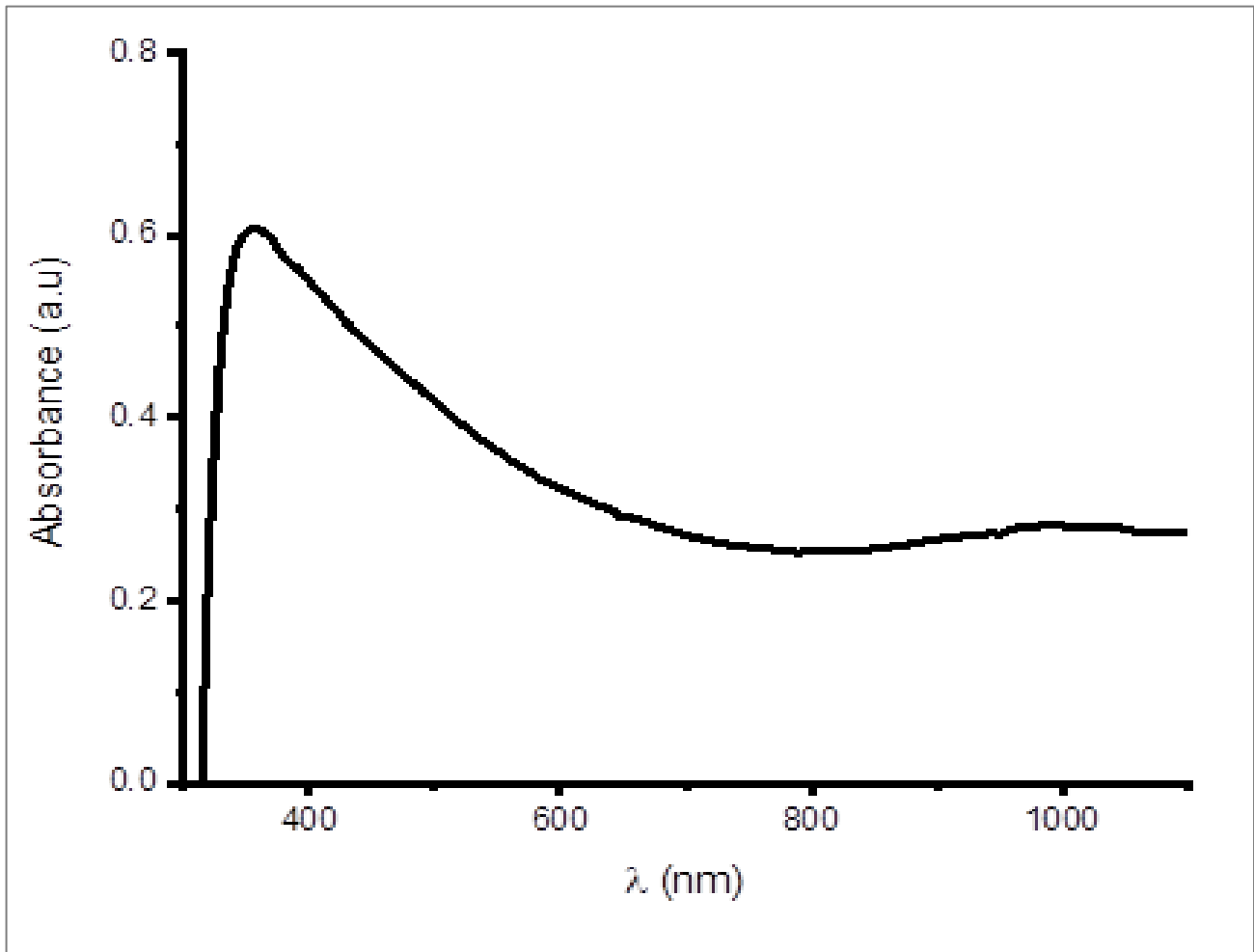


Figure 4: Optical absorption characteristics of CBFS thin film

The transmittance of the CBFS thin film was determined from Equation (6) (Efe et al., 2023; Okafor et al., 2025)

$$T = 10^{-A} \quad (6)$$

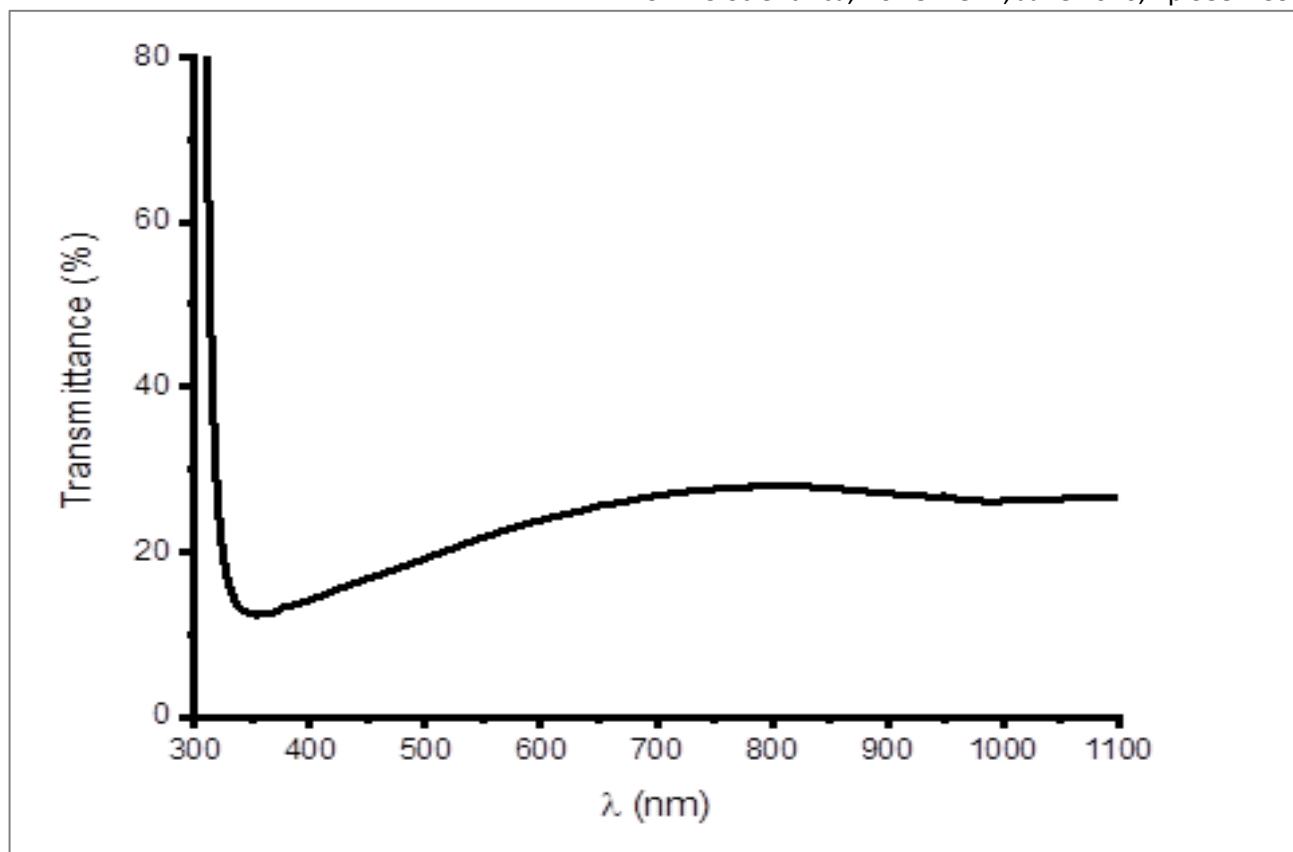


Figure 5: Optical transmittance characteristics of CBFS thin film

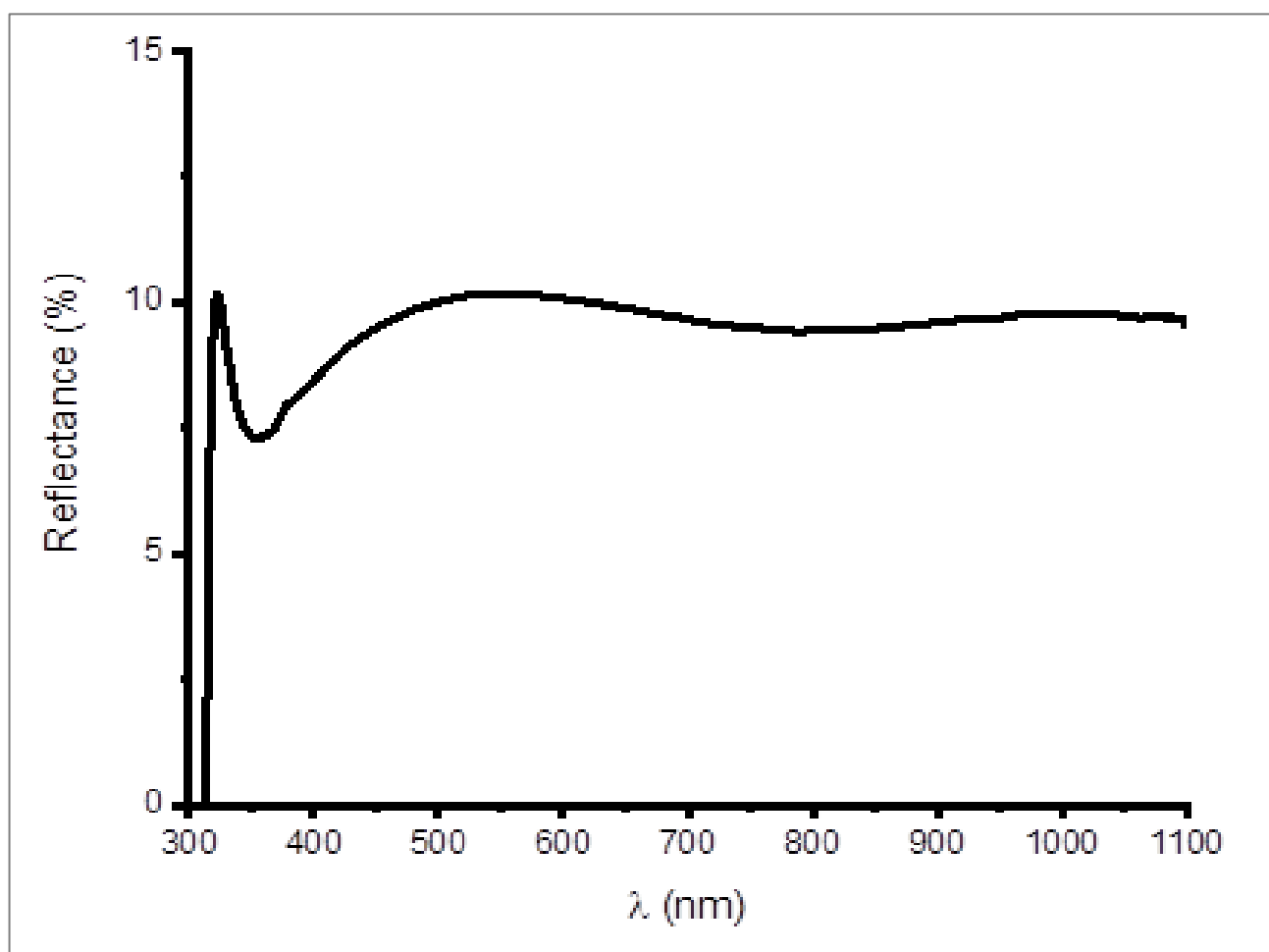


Figure 6: Reflectance spectrum of CBFS thin film

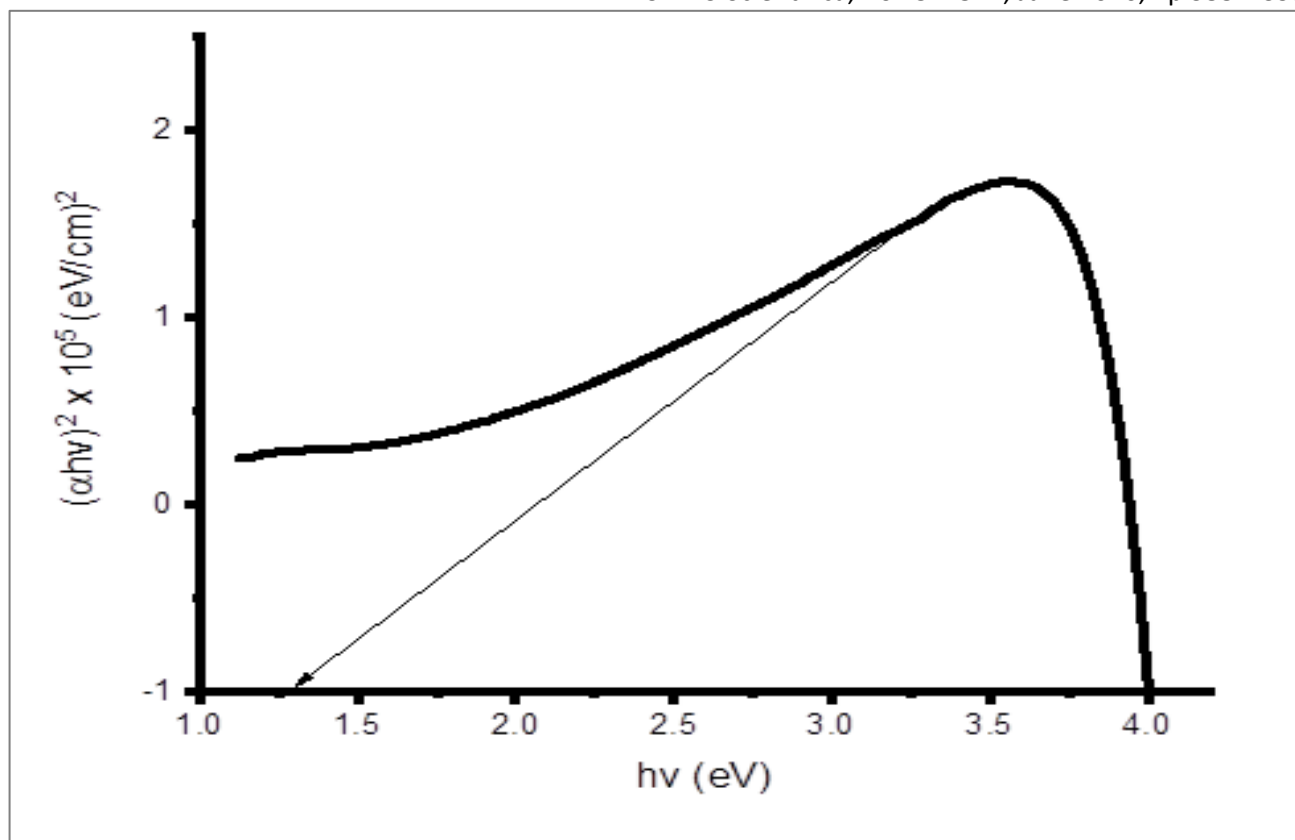


Figure 7: Square of absorption coefficient against energy for CBFS thin Film

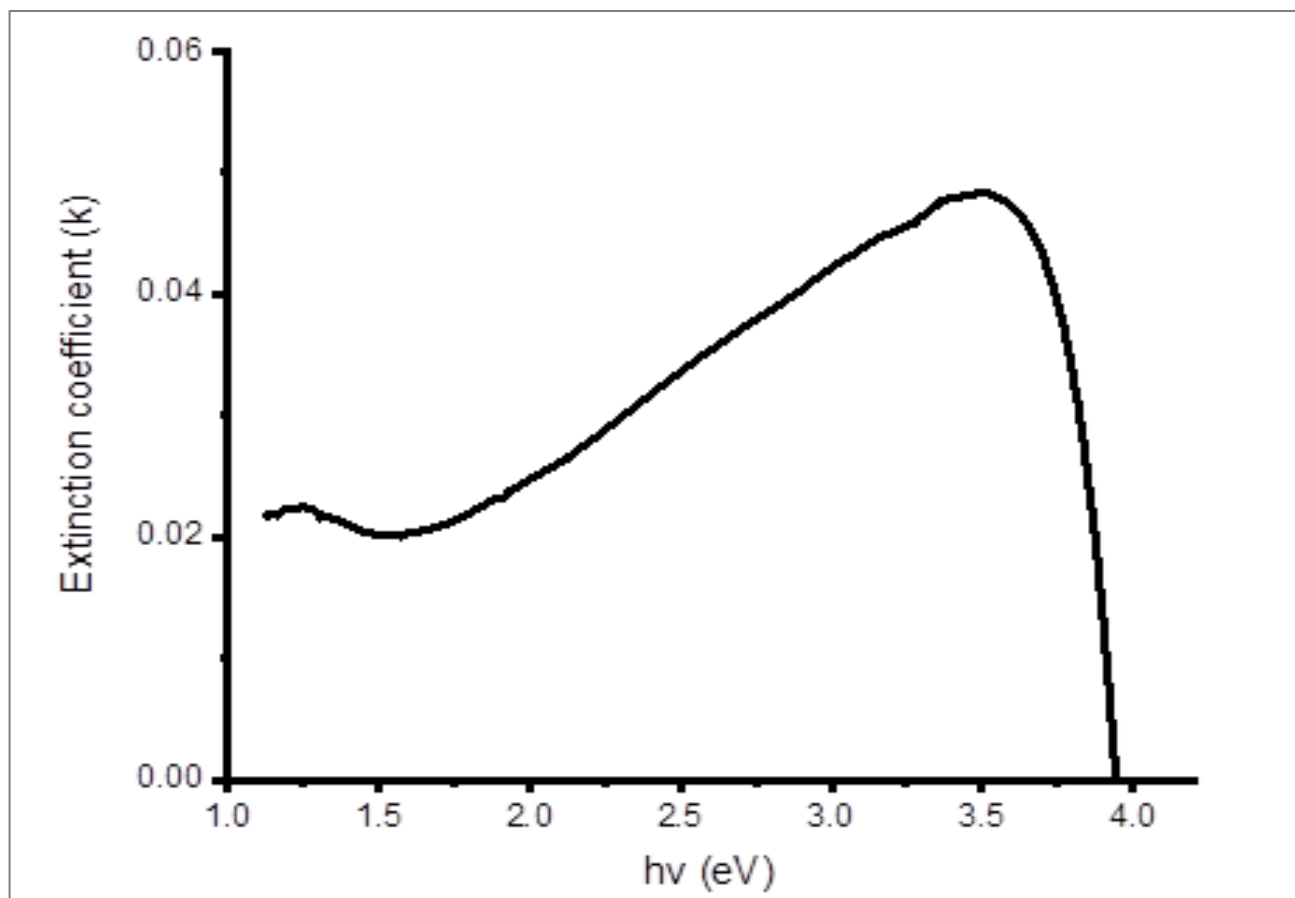


Figure 8: The extinction coefficient of CBFS thin films

Here, the absorbance is denoted as A. Figure 5 depicts the relationship between transmittance and wavelength for CBFS films. Across the entire range, the transmittance

was observed to increase from the visible to the near-infrared spectrum as the wavelength increased. Furthermore, the films exhibited a very low transmittance

of approximately 25% in the near-infrared region. Previous studies by [Nasrin et al. \(2024\)](#) have reported comparable findings. Appropriately, the low optical transmittance observed in this investigation may be

attributed to the nature of the chemical kinetics of the film's precursors, which consequently induces defects within the grain boundaries and diminishes the overall transmittance ([Cheng et al., 2017](#); [Nasrin et al., 2024](#)).

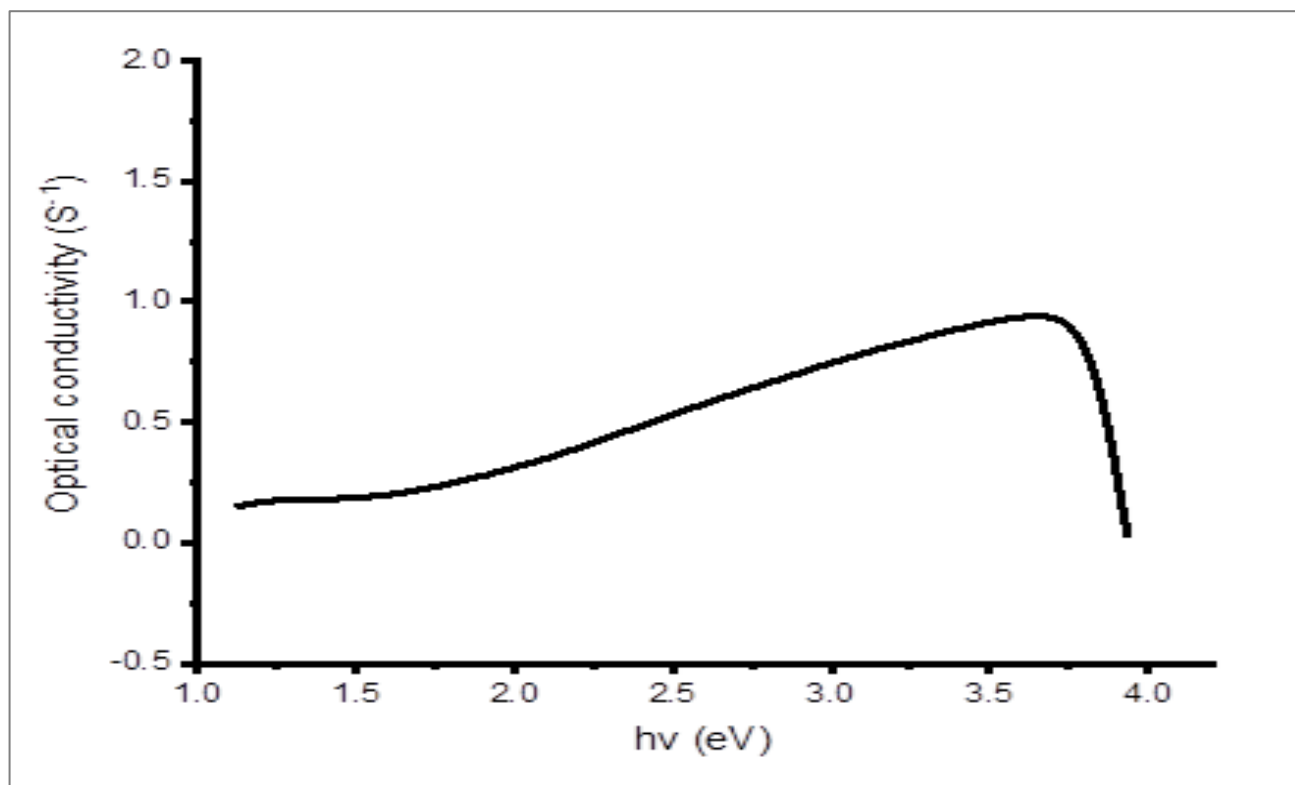


Figure 9: The optical conductivity of CBFS thin films

Table 1. Band gap energy of various quaternary thin films

Thin Film Composition	Band Gap (eV)	Reference
Ag-Zn-Sn-S	1.95 – 2.10	Yeh and Cheng, 2014
Cu-Zn-Sn-S	1.40	Zaki et al., 2021
Cu-Zn-Sn-Se	1.00	Botti et al., 2011
Cu-Fe-Sn-S	1.54	Rajeshmon et al., 2019
Cu-Ba-Fe-S	1.36	Present Work
Cu-Zn-Fe-S	1.50 – 1.96	Emegha et al., 2022

As depicted in [Figure 6](#), the reflectance of the deposited CBFS thin films exhibits a dependence on the wavelength, with the reflectance increasing as the wavelength increases. Generally, the samples have low reflectance values that lie between 0 and 10. However, at wavelengths exceeding 700 nm, the reflectance exhibits a quasi-parallel trend with the wavelength region. Similar observations for ternary copper chalcogenide thin films have been reported by [Emegha et al. \(2021\)](#). Consequently, the low reflective nature of the CBFS thin film makes it suitable for anti-reflective coatings material ([Babalola et al., 2024](#)).

The electronic band structure of thin film materials is the fundamental characteristic that governs the occurrence of direct optical transitions. The relationship between the energy of incident photons and the absorption coefficient is crucial for estimating the material's band gap energy, as detailed in the subsequent Equation (7) ([Damisa and Emegha, 2021](#))

$$\alpha = \frac{K}{h\nu} \int_{h\nu - E_g}^{\infty} \quad (7)$$

where the index z can take on values that depend on the type of electronic transition causing the absorption. Specifically, $z = 1/2$ for allowed direct transitions, $z = 2$ for allowed indirect transitions, $z = 3$ for forbidden indirect transitions, and $z = 3/2$ for forbidden direct transitions. Additionally, E_g represents the band gap energy, h is Planck's constant, ν is the frequency of the incident photon, and K is a constant independent of energy ([Damisa and Emegha, 2021](#); [Nwori et al., 2022](#)). The optical band gap was determined from a plot of the quantity $(ah\nu)^2$ as a function of photon energy ($h\nu$), which was derived from the preceding Equation (7) and the Tauc plot ([Nwori et al., 2022](#); [Guermat et al., 2022](#)). As shown in [Figure 7](#), a linear extrapolation of the plot of $(ah\nu)^2$ versus photon energy ($h\nu$) to the x-axis intercept at $\alpha = 0$ yielded a band gap energy value of 1.36 ± 0.05 eV ([Table 1](#)). The optical band gap energy value demonstrates that the CBFS thin film is a quaternary material, with a band gap that falls within the range of its binary and ternary components, thereby adhering to Vegard's law of mixture.

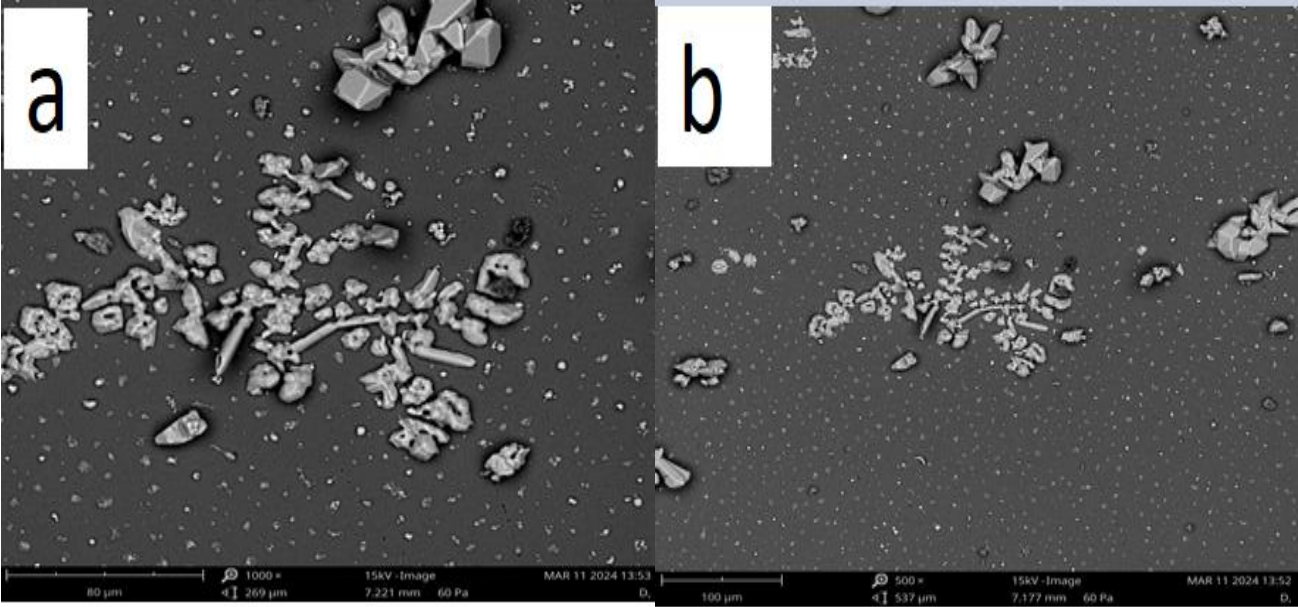


Figure 10: SEM images of CBFS thin film at various magnifications

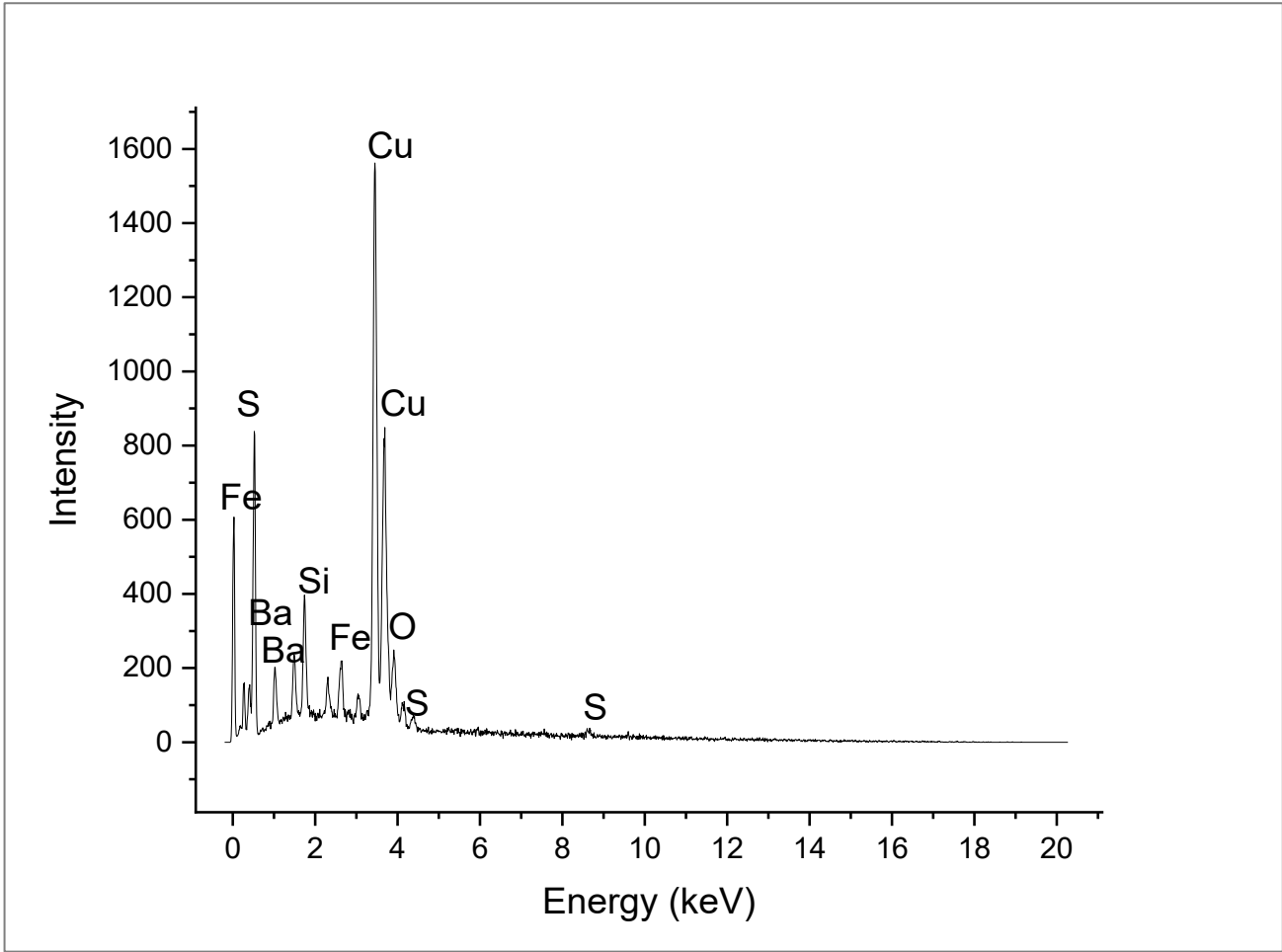


Figure 11. EDS spectrum of CBFS thin film

Table 2: Weight Concentration of CBFS Thin Films

Element Symbol	Element Name	Weight Conc. (%)
Cu	Copper	41.70
Ba	Barium	17.66
Fe	Iron	13.16
S	Sulphur	17.82
O	Oxygen	3.23
Si	Silicon	6.26

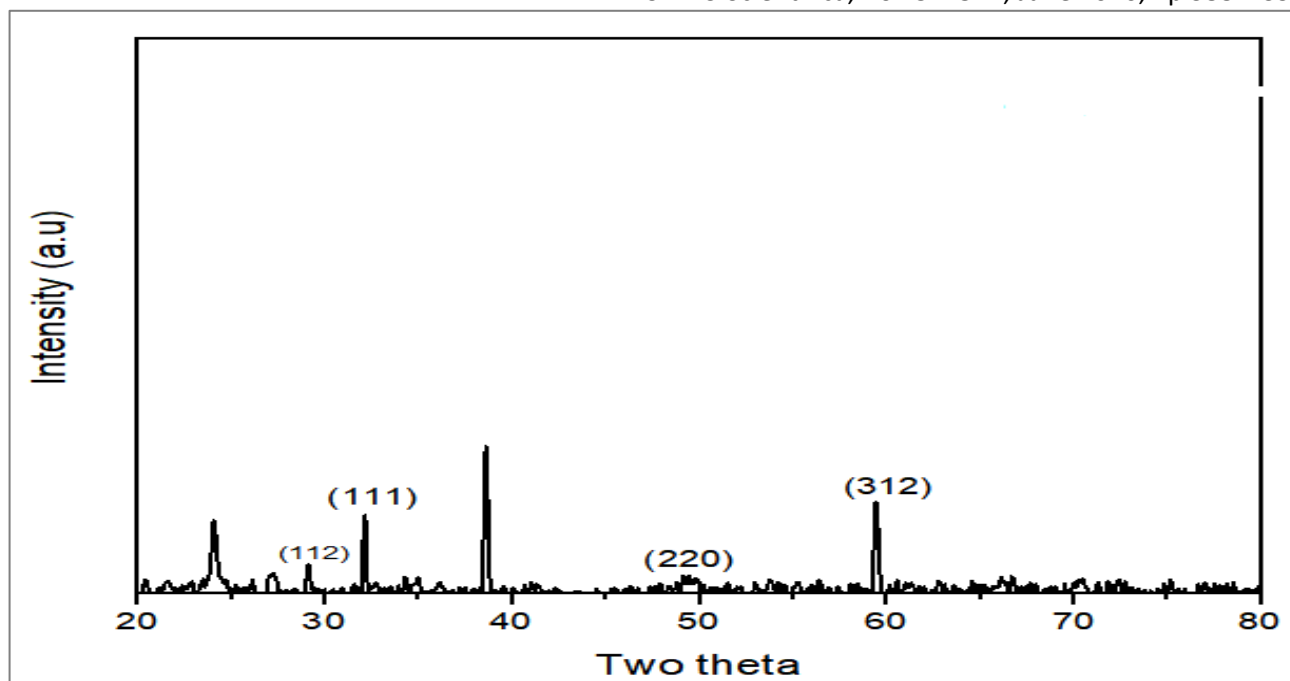


Figure 12: XRD pattern of CBFS thin film

Table 3: XRD Properties of CBFS Thin Films

(hkl)	2θ (°)	d-spacing (Å)	FWHM (°)	D (nm)	δ (lines/m ²)	ε (strain)
(112)	29.114	3.0647	0.2744	29.91	1.12×10^{15}	0.00473
(111)	32.133	2.7833	0.0610	135.53	5.44×10^{13}	0.00092
(220)	49.215	1.8499	0.1372	63.69	2.47×10^{14}	0.00143
(312)	59.472	1.5530	0.1029	88.91	1.27×10^{14}	0.00079

Key: D = Crystallite size; δ = Dislocation density; ε = Microstrain

Furthermore, the obtained band gap value of the CBFS thin film (as well as other quaternary thin films) indicated in Table 1 aligns with the band gap range (1.0 to 2.0 eV) of potential candidates for absorber materials considered suitable for solar cell applications (Ho and Anand, 2015; Chidozie et al., 2024). Different factors may cause the variations in band gap of the various quaternary thin films in Table 1. The band gap variations may be due to the nature of the grain sizes and crystallinity of the different thin film materials, which can lead to various degrees of variation in the localized states and strain (Damisa et al., 2017). Also, the band gap variation may be as a result of the difference in elemental composition, deposition time, temperature, concentration as well as the deposition process employed in the growth of the films. However, the values obtained in this study are slightly lower than the values reported by Rajeshmon et al. (2019), Zaki et al. (2021), and Emegha et al. (2022). The difference may be as a result of localized states in the material band.

The extinction coefficient (k) and the optical conductivity (σ) were determined using the mathematical expression as detailed in Equations (8) and (9) (Efe et al., 2019; Nwori et al., 2022)

$$k = \frac{a\lambda}{4\pi} \quad (8)$$

$$\sigma = \frac{amc}{4\pi} \quad (9)$$

where the wavelength of the incident photon energy is represented by λ, the speed of light is represented by c, and the absorption coefficient by α. As shown in Figure 8, the extinction coefficient of CBFS thin films varies with photon energy and exhibits fluctuations. The graph suggests that the average extinction coefficients of the material are generally low, indicating a correlation between the extinction coefficient and the transparent nature of the deposited films. This observed extinction coefficient behavior can be attributed to the successive internal reflections occurring within the film matrix (Emegha et al., 2021). The relationship between optical conductivity and photon energy is depicted in Figure 9. The graph clearly demonstrates that optical conductivity varies with photon energy. Specifically, optical conductivity rises from 0.2 S⁻¹ to a peak of 0.9 S⁻¹, then declines to zero as photon energy increases. The observed behavior can be attributed to the optical absorption characteristics of the films and the electron excitation phenomena occurring within the system as photon energy increases (Emegha et al., 2021).

The SEM micrographs of CBFS thin films at 80 and 100 μm magnifications are displayed in Figures 10(a) and (b). The micrographs reveal that the films consist of rounded, grain-like and micro-flowerlike distributed grains. The micrograph demonstrates the relationship between the compact surfaces and the various grains. This can also be explained by the smooth, as well as the irregular distribution of grains—either individually or in clusters—across the studied surface area. The film surface deposited

CONCLUSION

This paper presents for the first time the chemical bath deposition (CBD) technique to deposit copper barium iron sulphide thin films on glass substrates. This is a straightforward and economical technique suitable for the large-scale fabrication of thin films. Optical characterization demonstrated that the film possessed unique absorption and transmission properties, with variations observed across the wavelength spectrum. Featuring a band gap of 1.36 ± 0.05 eV, the material exhibits preliminary potential as a high-quality semiconductor for electronic device applications with comparable performance characteristics. Scanning electron microscopy images demonstrated well-covered nanostructured grains on the substrate surface, while X-ray diffraction confirmed the presence chalcopyrite crystal structures as the dominant phases in the films.

Future work should focus on the following:

- Applying Hall Effect measurements to determine the carrier concentrations, Hall coefficients, and mobility within CBFS thin films.
- Conducting electroluminescence and photoluminescence studies to reveal the luminescence properties of the films.
- Preparing and depositing quaternary CBFS thin films by varying deposition parameters and investigating their properties.
- Exploring alternative thin film deposition methods, such as sputtering and evaporation, to potentially produce higher-quality films

REFERENCES

- Abdullahi, S., Momoh, M., Moreh, A. U., & Wara, A. M. (2025). Preparation, characterization, and performance optimization of $\text{Cu}_2\text{ZnSnS}_4$ (CZTS) absorber layer deposited by sol-gel spin coating technique. *UMYU Scientifica*, 4(1), 1-18. [\[Crossref\]](#)
- Adebisi, A. C., Eluyemi, M. S., Emegha, J. O., Efe, F., Eleruja, M. A., & Olofinjana, B. (2025). Thermistor behavior of non-stoichiometric cadmium sulfide thin films. *Journal of Materials Science: Materials in Electronics*, 36, 1309. [\[Crossref\]](#)
- Akl, A. A., & Hassanien, A. S. (2021). Comparative microstructural studies using different methods: Effect of Cd-addition on crystallography, microstructural properties, and crystal imperfections of annealed nanostructural $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ thin films. *Physica B: Condensed Matter*, 620, 413267. [\[Crossref\]](#)
- Alam, A., Kumar, S., & Singh, D. K. (2022). Cadmium sulphide thin films deposition and characterization for device applications. *Materials Today: Proceedings*, 62, 6102-6106. [\[Crossref\]](#)
- Arun, A. P., Sreenivasan, N., Patil, J. H., Kusanur, R., Ramachandraiah, H. L., & Ramakrishna, M. (2025). Thin films for next generation technologies: A comprehensive review of

by CBD exhibits no signs of cavities or cracks within the substrates. Apparently, the coarse morphology is beneficial for photovoltaic generation, as the irregular edges capture more photons and enhance the absorption and current densities within the system (Emegha et al., 2022; Ikhiyoa et al., 2024).

The energy-dispersive spectroscopy (EDS) was employed to determine the elemental composition of the CBFS films deposited onto soda-lime glass substrates (Figure 11). The spectrum reveals the presence of copper, barium, iron, sulphur and other elements present in the glass substrate due to surface contamination (Owoeye et al., 2021). The characteristic composition of the films is presented in Table 2, as well as their atomic weight. From the elemental analysis, it was observed that the metals-to-sulphide ratios in the starting solutions were not preserved in the film. This may be attributed to the breakdown and successive reconstitution of the metal-metal-sulphide bonds during the deposition process. Hence, the result showed that the CBFS thin films are rich in cations. The results also showed that there is no trace of impurities such as carbon within the films (Damisa et al., 2017).

Figure 12 presents the XRD pattern of the CBFS thin film deposited over the range of 2θ from 10° to 80° . The observed peaks at 24.07° , 27.37° , 29.11° , 32.13° , 38.62° , 49.22° and 59.47° confirm the polycrystalline nature of the CBFS thin films. These peaks are consistent with the tetragonal chalcopyrite phase of CuFeS_2 , indicating that the deposited film is predominantly polycrystalline CuFeS_2 . No pronounced diffraction peaks corresponding to separate barium sulphide phases were observed, suggesting either successful incorporation of Ba into the CuFeS_2 lattice or the presence of Ba-containing phases below the detection limit of XRD. This trend may be attributed to surface reorganization within the films caused by the various elements within the Cu-Ba-Fe-S system. Similar observations have been reported in the literature for quaternary thin films (Nasrin et al., 2024).

The crystalline sizes (D), dislocation density (δ), and strain function (ϵ) of the deposited thin films were computed using Scherer's formulas, as shown in the Equations below (Akl and Hassanien, 2021; Elete et al., 2023):

$$D = \frac{0.9 \times \lambda}{\beta \cos \theta} \quad (10)$$

$$\delta = \frac{1}{D^2} \quad (11)$$

$$\epsilon = \frac{\beta \cos \theta}{4} \quad (12)$$

Where θ , β , and λ are the diffraction angle, full width at half maximum (FWHM), and the X-ray wavelength ($1.5406 \text{ \AA}$) respectively for the deposited copper-barium-iron-sulphide thin films. According to computational data, the crystalline sizes (D) varies from 29.91 to 135.52 (Table 3), depending on peaks location. Additionally, Table 3 shows that the dislocation density (δ) and strain (ϵ) of the deposited material also varies within the films, suggesting an improvement in the crystallinity of the thin films (Emegha et al., 2025).

- fundamentals, growth, deposition strategies, applications, and emerging frontiers. *Processes*, 13, 3846. [Crossref]
- Babalola, A. V., Oluwasusi, V., Owioye, V. A., Emegha, J. O., Pelemo, D. A., Fasasi, A. Y., Gurku, U. M., Alayande, S. O., Yusuf, S., & Saje, B. (2024). Effect of tin concentrations on the elemental and optical properties of zinc oxide thin films. *Heliyon*, 10, e23190. [Crossref]
- Botti, S., Kammerlander, D., & Marques, M. A. L. (2011). Band structures of $\text{Cu}_2\text{ZnSnS}_4$ and $\text{Cu}_2\text{ZnSnSe}_4$ from many-body methods. *Physical Review B*, 84(7), 075119. [Crossref]
- Cheng, J., Cao, G., Zong, H., Kang, C., Jia, E., Zhang, B., & Li, M. (2017). Highly transparent conductive AZO/Zr50Cu50/AZO films in wide range of visible and near infrared wavelength grown by pulsed laser deposition. *Results in Physics*, 7, 910-913. [Crossref]
- Chidozie, O. C., Nnanna, L. A., Akpu, N. I., Joseph, U., & Ikhioya, I. L. (2024). Study of the morphological, structural, electrical, and optical features of spray-deposited yttrium-doped magnesium selenide (YMgSe) thin film for photovoltaic applications. *Journal of Nano and Materials Science Research*, 3(1), 1-6.
- Damisa, J., & Emegha, J. O. (2021). Growth and optical analysis of cobalt tin sulphide thin films using SILAR technique. *Nigerian Research Journal of Engineering and Environmental Sciences*, 6(2), 642-648.
- Damisa, J., Olofinjana, B., Ebomwonyi, O., Bakare, F., & Azi, S. O. (2017). Morphological and optical study of thin films of CuAlS_2 deposited by metal organic chemical vapour deposition technique. *Materials Research Express*, 4(8), Article 086412. [Crossref]
- Efe, F. O., Olofinjana, B., Fasakin, O., Adebisi, C. A., Eleruja, M. A., & Fabunmi, T. G. (2023). Opto-electronic properties of copper-zinc-sulfide thin films grown via metalorganic chemical vapor deposition technique at different flow rates. *Physica Scripta*. [Crossref]
- Efe, F. O., Olofinjana, B., Fasakin, O., Eleruja, M. A., & Ajayi, E. O. B. (2019). Compositional, structural, morphological, optical and electrical property evolutions in MOCVD Cu-Zn-S thin films prepared at different temperatures using a single solid source precursor. *Journal of Electronic Materials*. [Crossref]
- Efe, F., Adebisi, A. C., Samokhvalov, A., Emegha, J. O., Achuko, N., Victor, M., Eleruja, M., & Olofinjana, B. (2026). Investigation of Cu-doped ZnS thin film: Optical, structural, and surface properties for potential thin film applications. *Results in Surfaces and Interfaces*, 100825. [Crossref]
- Elete, D. E., Emegha, J. O., Nenuwe, N. O., & Omagbemi, O. W. (2023). Synthesis and characterization of chemical bath deposited copper doped lead sulfide thin films. *Bulletin of the Chemical Society of Ethiopia*, 37(5), 1237-1251. [Crossref]
- Emegha, J. O., & Nwanze, E. D. (2022). Synthesis and characterization of semiconducting iron copper sulphide thin films: A review. *Physics Access*, 2(2), 18-24. [Crossref]
- Emegha, J. O., El-Rayyes, A., Itas, Y. S., & Khandaker, M. U. (2025). The impact of iron concentration on the structural and optical properties of iron lead sulphide thin films. *Journal of the Indian Chemical Society*, 102(10), 102085. [Crossref]
- Emegha, J. O., Okafor, M. C., & Ukhurebor, K. E. (2021). Optical properties of copper-zinc sulphide network from mixed single solid source precursors of copper and zinc dithiocarbamates. *Walailak Journal of Science and Technology*, 18(9), 1-11. [Crossref]
- Emegha, J. O., Ukhurebor, K. E., Aigbe, U. O., Damisa, J., & Babalola, A. V. (2022). Synthesis and characterization of copper zinc iron sulphide (CZFS) thin films. *Heliyon*, 8(8), e10331. [Crossref]
- Etim, E. E., Anas, H., Yakubu, S., Moses, L. J., & Samuel, H. S. (2025). Kinetics, thermodynamics, and isotherm properties of lead & silver metal ions removal from aqueous solution using tea leaves and tea fibers (*Camellia sinensis*). *UMYU Scientifica*, 4(1), 73-85. [Crossref]
- Fekadu, G. H. (2015). *Synthesis and characterization of cadmium selenide (CdSe) and lead sulphur selenide ($\text{PbS}_{1-x}\text{Se}_x$) thin films by chemical bath deposition method* [Doctoral dissertation, Kwame Nkrumah University of Science and Technology, Kumasi, Ghana].
- Guermat, N., Darenfad, W., Mirouh, K., Bouarissa, N., Kalfallah, M., & Herbadji, A. (2022). Effects of zinc doping on structural, morphological, optical and electrical properties of SnO_2 thin films. *European Physical Journal Applied Physics*. [Crossref]
- Ho, S. M., & Anand, T. J. S. (2015). A review of chalcogenide thin films for solar cell applications. *Indian Journal of Science and Technology*, 8(12). [Crossref]
- Ibrahim, A., Ado, A., Gabi, B., Abdul-Azeez, U. M., Bako, A. U., & Babagana, M. (2025). Phytogenic synthesis, structural elucidation and antiparasitic activity of *Ocimum gratissimum*-mediated silver nanoparticles against *Plasmodium falciparum* clinical isolate. *UMYU Scientifica*, 4(3), 427-436. [Crossref]
- Ikhioya, I. L., Alghamdi, N., Omeje, S. E., Ikeh, D. C., & Odoh, R. N. (2024). Synergistic effects of gadolinium oxide into the matrix of zeolitic imidazolate frameworks (ZIFs) for supercapacitor applications. *Chemistry of Inorganic Materials*, 4, 100075. [Crossref]
- Llorens Balada, E. (2024). *Metal oxide thin films for optoelectronic applications* [PhD thesis, DTU Nanolab].
- Nasrin, R., Khan, L., Obaydul Haq, M., Mohiuddin, M., & Kabir, H. (2024). Surface topography, structural, optical and DC electrical behaviors of pristine and Co-doped ZnS thin films. *Heliyon*, 10(8), e29337. [Crossref]

- Nwori, A. N., Okoli, N. L., Okereke, N. A., Ottih, I. E., & Ezenwaka, L. N. (2022). Optical properties of electrodeposited CdMnS thin film semiconductor alloys for optoelectronics applications: Effect of deposition potential. *Journal of Nano and Materials Science Research*, 1, 58-67.
- Okafor, M. C., Esiekpe, L. E., Attah, V. A., Okeke, N. B., Okwuelum, A. B., & Emegha, J. O. (2026). Optimization of copper ion concentration into the lattice of barium sulphide nanoparticles synthesized via a chemical approach. *Journal of Theoretical and Applied Physics*, 20(2), 185-195. [\[Crossref\]](#)
- Owoeye, S. S., Abegunde, S. M., Folorunso, D. O., Adigun, B. O., & Kingsley, U. (2021). Microstructure, phase and physical evaluation of non-bioactive wollastonite glass-ceramic prepared from waste glass by sintering method. *Open Ceramics*, 5, Article 100062. [\[Crossref\]](#)
- Palazon, F. (2022). Metal chalcogenides: Next generation photovoltaic materials? *Solar RRL*, 6, 2100829. [\[Crossref\]](#)
- Rajeshmon, V. G., Kartha, C. S., Vijayakumar, K. P., Abe, T., Kashiwaba, Y., & Kunjomana, A. G. (2019). Growth and characterization of spray deposited quaternary Cu₂FeSnS₄ semiconductor thin films. *Physica B: Condensed Matter*, 560, 103-110. [\[Crossref\]](#)
- Sarf, F., Yakar, E., & Karaduman Er, I. (2024). Thin films: Growth, characterization and electrochemical applications. *IntechOpen*. [\[Crossref\]](#)
- Shepelin, N. A., Tehrani, Z. P., Ohannessian, N., Schneider, C. W., Pergolesi, D., & Lippert, T. (2023). A practical guide to pulsed laser deposition. *Chemical Society Reviews*, 52, 2294. [\[Crossref\]](#)
- Turnley, J. W., & Agrawal, R. (2024). Solution processed metal chalcogenide semiconductors for inorganic thin film photovoltaics. *Chemical Communications*, 60, 5245. [\[Crossref\]](#)
- Yahaya, A. A., Umar, A. B., Mamuda, S., & Ahmad, A. M. (2022). Characterization of the structural and optical properties of copper oxide for use in solar cells using screen printing method. *UMYU Scientifica*, 1(1), 184-193. [\[Crossref\]](#)
- Yeh, L. Y., & Cheng, K. W. (2014). Preparation of Ag-Zn-Sn-S quaternary photoelectrodes using chemical bath deposition for photoelectrochemical applications. *Thin Solid Films*, 558, 289-293. [\[Crossref\]](#)
- Zaki, M.-Y., Sava, F., Buruiana, A.-T., Simandan, I.-D., Becherescu, N., Galca, A.-C., Mihai, C., & Velea, A. (2021). Synthesis and characterization of Cu₂ZnSnS₄ thin films obtained by combined magnetron sputtering and pulsed laser deposition. *Nanomaterials*, 11(9), 2403. [\[Crossref\]](#)
- Zhu, H., Zhang, W., Zhao, K., Jin, C., Zhang, Z., Xu, K., Liu, Y., Wang, J., & Saetang, V. (2025). Recent advances in precision deposition techniques on semiconductor surfaces: Mechanisms, methods, and applications. *Materials Today Communications*, 48, 113495. [\[Crossref\]](#)