IOSR Journal of Applied Physics (IOSR-JAP)
e-ISSN: 2278-4861.Volume 14, Issue 1 Ser. III (Jan. – Feb. 2022), PP 25-29
www.iosrjournals.org

Phytochemical, Optical and FTIR Studies of ZnSe Thin Films for Solar Energy Applications

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Abstract
Zinc selenide thin films were successfully deposited on a glass substrate at 333K and 353K using chemical bath technique by an aqueous mixture appropriate percusors to provide the needed Information Znic ion and selenide ion. The dye extracted from the leaf of zea maze (maize) plant was used to sensitize the film. Uv spectrophotometer was used in the optical analysis. Fourier infra red transform was used to determine the absorption peaks of the films corresponding to different functional groups. The phytochemical and FTIR analysis of the films revealed the presence of primary photoreceptors like phenol (O-H Strength, H-bonded), carotenoids and alkanoids (C-H strength) at 3235cm^{1} and 3390cm^{1} respectively. The results indicated that the addition of dye and increase in deposition temperature has a profound influence on the optical properties of the deposited films. The absorbance spectra indicated that all the deposited films were absorbing in the visible region at different maxima wavelength of 300nm to 450nm because of the carotenes and Xanthophylls in the dye. There was a gradual increase in the extinction coefficient of the films towards the higher photon energy.

Keywords: *Phytochemical, Extimction coefficient, chemical bath, FTIR, dye, Absorbance, UV–Spectrophotometer, Temperature and annealing.*

Date of Submission: 01-02-2022 Date of Acceptance: 13-02-2022

I. Introduction

In this modern world energy has become an integral part of our life; its supply should be secure and sustainable. The energy requirement of the world is ever increasing. The increasing energy demands put a lot of pressure on the conventional energy sources. Therefore, there is a need for alternative energy sources which can provide us energy in a sustainable manner. The obvious choice of a clean energy source, which is abundant and could provide security for the future development and growth, is the sun's energy. In this 21st century, the use of solar energy powered devices ranging from hand held to more bulky and installed ones are very common occurrence [5]. There have been immense improvements in solar Technology such that its development and refining is capable of powering thousands of installations worldwide.

Solar electricity was once considered an exotic technology but was only given attention in terms of powering space satellites and an occasional classroom experiment [2, 6]. Solar electricity can power anything from calculator to an entire community. Today, solar electricity has become practicalised and hence applied as a means of generating electricity outside power lines. They have no moving and maintenance parts with long life span exceeding for decades. Photovoltaic are these days standardized such that its application is extended to many commercial, industrial, military as well as other consumer applications for modest power requirements [3, 2]. Dye-sensitized solar cells (DSSC) are promising alternatives to conventional solar cells because of their cheap, environmentally friendly, and easy to fabricate [12, 3]. Dye-sensitized ZnSe thin film because of its panchromatic nature has been found useful in solar energy harvesting. They work even in low-light conditions such as non-direct sunlight and cloudy skies.

Thin film technology has provided an opportunity for investigators to delve into solar energy research [2, 13]. Zinc Selenide (ZnSe), a group II-IV semiconductor compound has gained a remarkable attention in solar energy device fabrication due to its good optical and solid state properties [5]. It is a leading material in the fabrication of solar cells. It has direct band gap transition type [7, 9]. ZnSe is a preferred material for lenses [2, 3, 5], window layers and output couplers for its low absorptive at infra-red wavelengths and its visible transmission [3, 5]. Nano based zinc selenide thin films with a wide direct band gap (3.87) has a high transmittance in the visible region having great interest in practical applications in optoelectronics and photonic [7, 9]. Dye-sensitized ZnSe thin films can be deposited using a variety of methods, including thermal evaporation, self assembly technique, spray pyrolysis, electron beam evaporation, and solution growth technique.etc [2, 1]. In this present work, dye-sensitized ZnSe thin films were deposited using chemical deposition technique and annealed. The samples were characterized using Spectrophotometer and Fourier infra red transform.

II. Experimental Detail

Chemicals used in this work were analytical grade (AR) and the solutions were prepared in deionized water. The chemical bath used to prepare dye-sensitized ZnSe thin films in this work were prepared in the following order. 20ml of 0.7M ZNSO4, 20ml of 0.3M CH4N2S, 2drops of NH3 and 4ml of Dye was added in 100ml cleaned and dried beaker labeled (1). 20ml of 0.7M ZNSO4, 20ml of 0.3M CH4N2S, 2drops of NH3without dye was also added in 100ml cleaned and dried beaker labeled (2). The pH level of beaker (1) content was 9.0 and reduced to 8.9 on addition of 4ml of dye. The content of beaker 1 and 2 was stirred for about five minutes to ensure proper mixture, thereafter; substrates separated and suspended with synthetic foam were immersed vertically at the center of each reaction bath (i.e. 100ml beaker 1 and 2). These reaction baths was inserted in water bath (1000ml beaker containing about 400ml of water) and was heated with constant temperature magnetic stirrer. The substrates used for the deposition of dye sensitized ZnSe thin films were microscopic glass slide (25.4mm x 76.2mm) already prepared. The films were deposited at constant temperature of 800C for 60minutes. The process was repeated with 20ml of 0.5M ZNSO4 and the films deposited at constant temperature of 600C for 60minutes.

III. Results and Discussion

Optical Characterization

Absorbance is the quantity directly determined from absorption spectra measurement and the instrument scales are often calibrated in this unit (au). As light passes through the interface between two different materials such as thin film and glass, a fraction of light is reflected by the inner surface while some amount of electromagnetic wave is refracted through the inner surface and finally transmitted. The reflectance is the amount of reflection in terms of energy while transmittance is the amount of transmission in terms of energy. Mathematically, by definition, Absorbance is

$$A = \log\left({}^{I_O}/_{I}\right) = log_{10}\left({}^{I}/_{T}\right) \qquad 1a$$

$$A = 2 - log_{10}(\%T) \qquad 1b$$

Where I_O and I are the incident and transmitted intensities respectively. According to [4, 5], absorbance and absorption coefficient (a) are related thus;

$$a \quad = \frac{Ac}{V} \qquad 2$$

Where c, and v are the velocity of light and frequency of the electromagnetic wave respectively. Absorbance can be calculated from transmittance or % transmittance using equation 1a and 1b. It is the absorbance/transmittance of thin films that are usually obtained directly using spectrophotometer during optical characterization while other properties are gotten from calculations based on these.

The Transmission spectra of the dye sensitized ZnSe thin film samples are taken in the ultra violet (UV), visible and infra red (IR) regions (200-900nm) by using UV-VIS-NIR Perker Elmer spectrophotometer lambda 950 with UV Win lab software. The machine measures directly the transmission of the sample. By using the %T data, all other optical parameters were calculated. The absorbance value for all the deposited dye-sensitized ZnSe thin films at different temperatures was displayed in Fig. 1. The plot indicated that all the deposited ZnSe thin films are absorbing in the visible region of the spectrum at different maxima wavelength between 300nm and 450nm. This could be ascribed to the presence of primary photoreceptors – phenol, carotenes, Tanin, and Xanthophylls in the dye as revealed by the phytochemical and FTIR analysis and due to the antioxidant properties of Xanthophylls the plot indicates that deposited dye-sensitized ZnSe thin films have its absorbance value decreased with increased wavelength. Its highest value recorded was 0.59 for film deposited at 353k and the lowest 0.13 for film deposited at 333k. Also noticeable was that increase in deposition temperature increased the absorbance of the films.

The Extinction coefficient (k) for a particular substance is a measure of how well it absorbs electromagnetic radiation. It is also a measure of light loss due to scattering and absorption per unit volume. If the EM wave can pass through very easily, the material has a low extinction coefficient. Conversely, if the radiation hardly penetrates the material, but rather quickly becomes "extinct" with it, the extinction coefficient is high. A material can behave differently for different wavelengths of electromagnetic radiation. Extinction coefficient generally depends on incident wavelength and is widely used in ultraviolet-visible spectroscopy.

Extinction coefficient can be expressed as;

$$K = \frac{a\lambda}{4\pi} \quad 3$$

Where a is absorption coefficient and λ is wavelength.

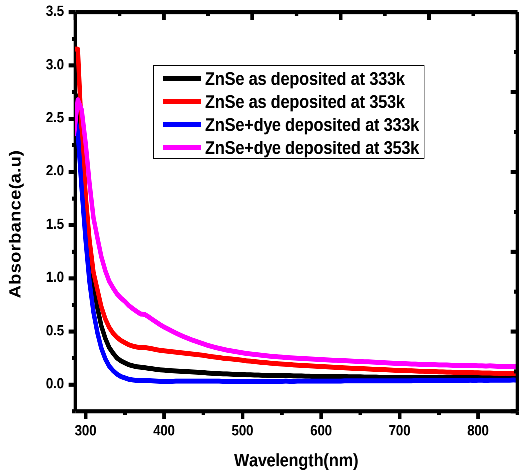

Fig: 1 plot of Absorbance versus wavelenght for dye sensitized ZnSe thin films

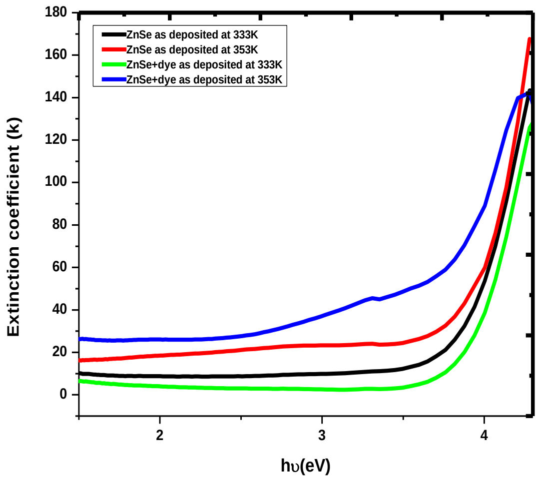

Fig: 2 plot of Extinction coefficient versus photon energy for dye sensitized ZnSe thin films

The plot of extinction coefficient against photon energy for the deposited ZnSe thin films with and without dye was shown in Fig.2. The value k was calculated using equation (3). A gradual increase in the k value towards the higher photon energy value was observed. The increase showed the strong absorbing (optical energy) nature of the deposited thin films. This value was in agreement with [4]

Phytochemical analysis:

Qualitative and quantitative analysis of the plant extract (dye) used in this study was done using Gas Chromatography- Mass Spectroscopy (GCMS). The Phytochemical screening revealed the presence of Terpenoids, Lycopene, Alkanoids, Phytate, Oxalate, Flaronoids, Tanin, Xanthophylls, Phenol, and Carotenoids as displayed in the bar chart below in the order of their increasing magnitude. From the chart, Carotenoids, phenol (Hydroxyl group -OH), Xanthophylls and Tanin are the most abundant pigments in the extract. These abundant parameters function as primary photoreceptors (light receptor molecule that respond to changes in light intensity, quality, direction and duration). Carotenoids have the highest value followed by phenol while the least is terpenoids. Many of the Carotenes (orange) and Xanthophylls (yellow) absorb in the wavelength range of 425 to 475nm. Beta-carotene has the highest absorption at 450nm while xanthopylls, lutein and vioxanthan absorb the most at approximately 435nm. Phenols and alkanoids as confirmed in FTIR spectra of Figs. 4 and 5 absorbs at 3235nm and 2850nm, with this there is a good percentage of agreement between the phytochemical and FTIR analysis of the dye used.

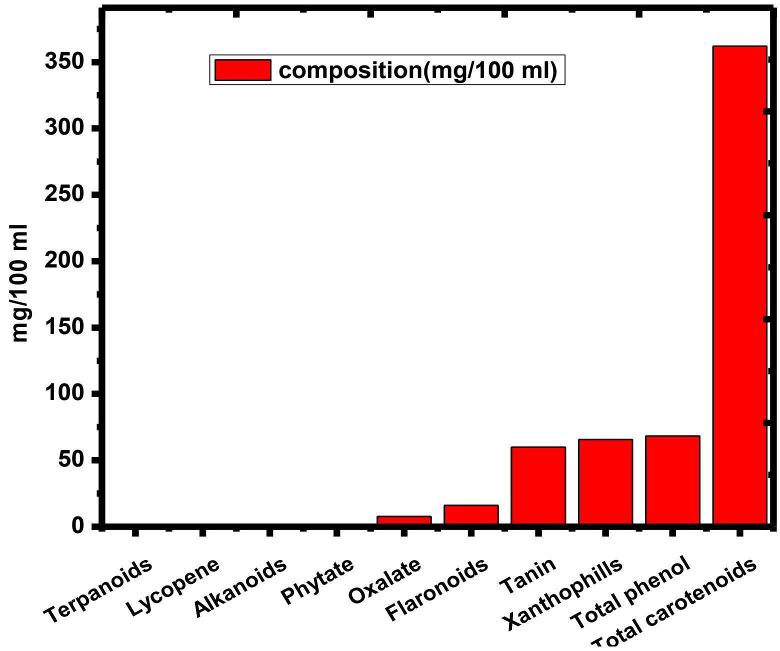

Fig: 3 Bar Chart of the Phytochemical compositions of the dye

FT-IR analysis:

An infrared spectrum of absorption or emission of a solid, liquid or gas is obtained using Fourier–transform infrared spectroscopy (FTIR) technique. The name Fourier transform infrared spectroscopy originates from the fact that a Fourier transform (a mathematical process) is required to convert the raw data into the actual spectrum. An FTIR spectrometer simultaneously collects high-spectral resolution data over a wide spectral range i.e. it measures and records the whole spectrum instead of just a region limited by resolution as dispersive spectrometers. It is used to decompose the light beam into its Fourier components. Fourier Transform Infra red (FTIR) measurements have been carried out to identify organic and/or inorganic chemical present in the sample, which is attributed to different functional groups corresponding to different absorbance peaks in the spectra. When the sample is irradiated by infrared light there is a transition between two transitional levels (found from schrodinger equation), manifesting the molecules present in the sample [8]. The FT-IR transmission spectrum of dye sensitized ZnSe thin film in the range of interest (1000-4000nm) is displayed in Figs: 4 and 5.

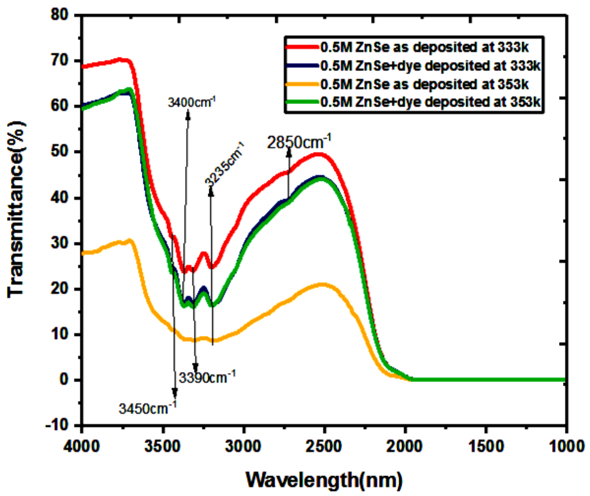

Fig. 4: FTIR spectra of 0.5M dye-sensitised ZnSe thin films

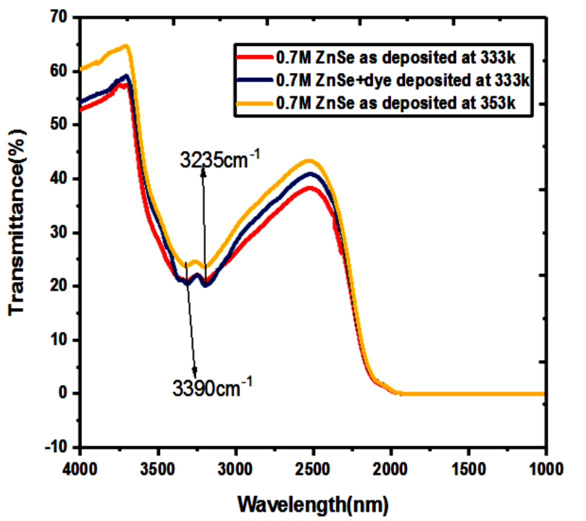

Fig. 5: FTIR spectra of 0.7M dye-sensitised ZnSe thin films

Figure 4 and 5 shows the FTIR spectra of deposited dye-sensitised ZnSe thin films at different moles. A series of absorption peaks were observed from 3200 to 3500nm. A strong and broad peak was obtained at 3235nm indicating the presence of hydroxyl group (O-H stretch, H-bonded) which could be attributed to the ability of the dye component like phenol to form intermolecular hydrogen bonds easily with water and also due to easy electrophilic aromatic reaction associated with phenol, xanthophyll and tanin in the dye. Another strong and broad peak present in the spectra at 3390nm is due to C-H stretch. Here, we have found impurities like hydroxyl (O-H) and Alkyne (C-H). Hydroxyl group may be generated in the sample due to the reaction of ZnSe with the dye or HCL used in cleaning the apparatus. The alkyne group can be produced due to acetone (CH_3COCH_3) wash of the oxidized wafer.

IV. Conclusions

In this study, Phytochemical, Optical and FTIR analysis of ZnSe thin films deposited on glass substrate using solution growth technique have been carried out. The phytochemical and FTIR studies of the films in agreement revealed the presence of many primary photoreceptors. The analysis showed that the addition of dye and increase in deposition temperature increased the absorbance of the films. The high absorbance of the deposited thin films indicated that dye sensitised ZnSe can be used in solar cell fabrication as an absorber.

References

[1]. Abeles, F. (1972). Optical properties of Metals and Solids. Amsterdom, North Holland Publishing Company, 97.

[2]. Agbo, P. E., Nwofe, P. A., & Odo, L. O. (2017). ANALYSIS ON ENERGY BANDGAP OF ZINC SULPHIDE (ZnS) THIN FILMS GROWN BY SOLUTION GROWTH TECHNIQUE. Chalcogenide Letters, 14(8).

[3]. Agbo, P. E. and Nwofe, P. A. (2015). Structural and Optical properties of Sulphurised Ag_2S thin films. International journal of thin Films Science and Technology, 4, 9-12.

[4]. Agbo, P. E. and Nwofe, P. A. (2015). Comprehensive studies on the Optical properties of ZnO-core. Journal of Nanotechnology Advance Material, 3, 63-97.

[5]. Ben Joshua Robert, Nworie Ikechukwu and Agbo P.E (2022)."Effects of Dye on Selected Optical and Solid State Properties of ZNSE Thin Films for Applications in Solar Energy Harvesting Device."IOSR Journal of Applied Physics (IOSR JAP), 14(01), 2022, pp. 01-04.

[6]. Chopra, K. L. and S. R. Das, 1983. Why Thin Films Solar Cells? Springer.

[7]. Dexter, D. L. (1956). Absorption of light by Atomsin Solids. Physical Review latters, 101, 48-55.

[8]. P. E. Agbo, P. A. Nwofe, C .A Elekakwachi , M . N Nnabuchi . J .Ovonic Res. 12 (3) ,163-1169 (2016)

[9]. Ismail, B. and R. Gould, 1989. Structural and electronic properties of evaporated thin films cadmium telluride. Physica Status Solidi (A), 115 (1): 237-245.

[10]. Molyneux, R. J., Lee, S. T., Gardner, D. R., Panter, K. E., James, L. F (2007)."Phytochemicals: the good, the bad and the ugly?". Phytochemistry. 68 (22–24): 2973–85.Doi: 10.1016/j.phytochem.2007.09.004. PMID 17950388.

[11]. Moss, T. S. (1961). Optical Properties of Semiconductors. London, Bullenworth and Co. Publishing Ltd, 2.

[12]. Nazar, A.S. (2014). Physical Properties of Silver Doped ZnSe Thin Films for Photovoltaic Applications. Iranian Journal of Energy and Environment 5 (1): 87-93, 2014

[13]. Nwofe, P. A., Robert, B. J., & Agbo, P. E. (2018). Influence of processing parameters on the structural and optical properties of chemically deposited Zinc Sulphide thin films. Materials Research Express, 5(10), 106405.

[14]. Okoli (2007). Growth and Characterization of Ternary Compounds and Possible Applications. Ph.D Thesis, Department of Physics and Industrial Physics NAU Awka

[15]. Onah, D. U., Agbo, P. E., Nwodo, M. O., Ijeh, R. O., Uguru, E. H., & Omeje, C. U. (2021). Thermal

[16]. Annealing On the EDS and Optical Properties of TiO 2/CuO Core-Shell Thin Films. European Journal of Material Science, 8(2), 1-9.

[17]. Thewlis, J. (1962). Encyclopaedic Dictionary of physics. Oxford Pergamann Press, 5, 1179.

[18]. Tiwari, G. N. (2012). Solar Energy Fundamentals, Design, Modeling and Applications. New Delhi, India: Nasora Publishing House Pvt. Ltd.

Nworie Ikechukwu Christian, et. al. "Phytochemical, Optical and FTIR Studies of ZnSe Thin Films for Solar Energy Applications." *IOSR Journal of Applied Physics (IOSR-JAP)*, 14(01), 2022, pp. 25-29.