Optical Examination on Zinc Sulphide Nanoparticles for Photovoltaic Applications

P Sharmili, M S Revathy, S Rajesh, M Muthu Vinayagam, R Chokkalingam

Abstract*: In this research work Zinc Sulphide nanoparticles are synthesized by co–precipitation method with zinc nitrate and sodium sulfide sources. The obtained particles are characterized to know its structure, crystalline pattern, crystalline size and other morphologies. The crystalline size of the material is calculated by Debye–Scherrer Formula. X–Ray Diffraction analysis, Scanning Electron Microscopy, Fourier Transform Analysis and UV–Visible spectrum analysis is performed to study the mentioned morphology and properties of the material synthesized. The central point of this research work is to study the behavior of Zinc sulfide nanoparticles for solar cell applications. Hence, luminescence property of the material is finally analyzed.

Keywords: About four key words or phrases in alphabetical order, separated by commas.

I. INTRODUCTION

Zinc sulphide has long been widely used in various fields of science and technology. However, interest in zinc sulphide is increased when it is known to develop new nanomaterials with unique properties. Zinc sulfide is a wide-band-gap semi-conductor with a range of potential applications in optoelectronic devices [1]. The use of nano-materials as composites are gaining importance in science and technology owing to their superior properties like thermal, electrical conductivity, optical, photoluminescence and other novel attributes [2]. The ZnS material is an intrinsic semiconductor with wide band gap of about 3.54eV for cubic and 3.91eV for hexagonal form[3]. As a wide band gap semiconductor, ZnS is a promising candidate for replacement of toxic cadmium sulfide (CdS) in the thin film solar cell application [4]. ZnS is an important material for diverse optoelectronic device applications such as sensors, electro-optic modulators, n-type window layers in photovoltaic cells, and electroluminescent devices.

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Though we have enormous types of solar cells everything does not possess energy efficiency. Still, solar cells possess high heat absorbance since energy from sunlight heats up the panel. Increase in the thermal energy decreases the efficiency of solar cells. Investigation on Photovoltaics (PV) attracted many researchers since their growing demand. Regarding efficiency of solar cells, the aim for detection and conversion of solar light into electrical energy at the atomic level was investigated broadly [5, 6]. Window materials layers have also been alternatively used as an effort to decrease the loss of absorption in the window layer [7]. The highest reported values of power conversion efficiencies (PCEs) for pure CZTS, pure CZTSe and their mixture based solar cells have reached 8.4, 12.6 and 11.6%, respectively [8, 9]. The maximum efficiency recorded for copper indium sulfide (CuInS2) thin-film based solar cell is 12.5% and in the case of using ZnS the best efficiency of about 7.8%, was recorded for the cell structure Mo/CuInS2/ZnS/ZnO [10].

In this study, to understand the importance of absorbance and luminescent parameter for ZnS materials using simple synthesis technique. The main objective of this work is to investigate the photoluminescent and thermoluminescent characteristics of ZnS experimentally.

II. EXPERIMENTAL WORK

The precursors are zinc nitrate Zn(NO3)2 for Zinc source and Sodium sulfide Na2S for Sulphide source. 0.1M of Zinc Acetate was prepared in ethanol and 0.1M sodium sulfide solution was taken in a burette. Under controlled addition of sodium sulfide drops to Zinc acetate solution and constant stirring for 12 hours, a white precipitate was obtained. The precipitate was centrifuged and sonicated using ultrasonic cleaner and washed 4 to 5 times with deionized water. The precipitate was dried in muffle furnace at 200℃ for 4 hours. Then, the obtained powder sample was stored for further characterization studies. The procedure was repeated for the concentration of ZnS 0.2M till1M.

III. RESULTS AND DISCUSSION

A. XRD Pattern of ZnS Nanoparticles:

The arrangement of atoms in a crystal plays a vital role in defining the properties of a material. Almost all the properties depend on the structure of a material. For example, Diamond and Graphite are allotropes of carbon.

As we know diamond is the strongest material whereas graphite is brittle and we can easily break the graphite material.

The structure of ZnS Nano particles were characterized by using X-Ray Diffractometer. The results obtained were compared with JCPDS data and peaks were indexed as per the JCPDS profile.

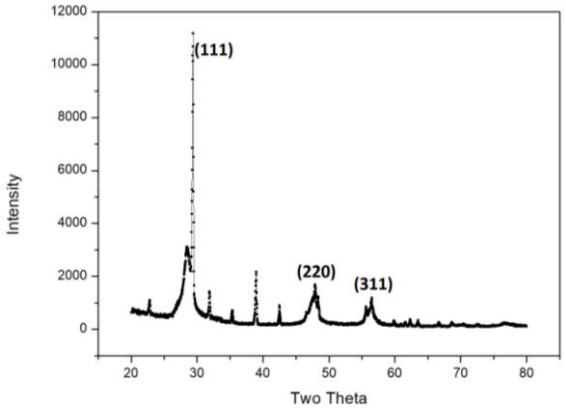

Fig 1. XRD pattern for 0.1 M concertation ZnS

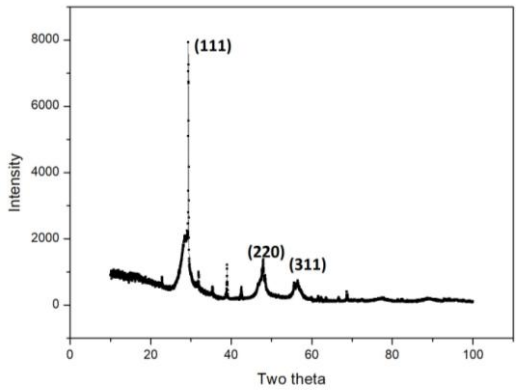

Fig 1. XRD pattern for 0.2 M concertation ZnS

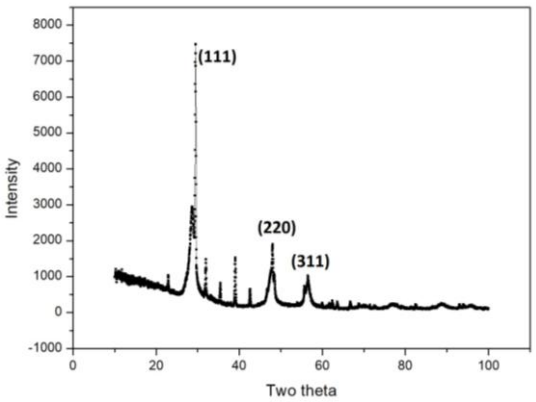

Fig 1. XRD pattern for 0.3 M concertation ZnS

The crystalline nature of the prepared nanosized ZnS powder is evident from the X-ray diffraction pattern Fig. 1. The indexed peaks at 2θ = 19.409˚, 2θ = 27.786˚, 2θ = 33.053˚ and 2θ = 33.521˚ corresponding to the (111), (220) and (222) planes, respectively, matches with the reported value (JCPDS card, No. 5-0566). The peaks are identified as spherically cubic (blend) structure. The broad feature of the peaks indicates the crystal size is in nanometers range. The isostructural phase may be caused by the presence of substitutional impurities of similar atomic size but differing atomic number that give rise to deviation in intensity.

XRD patterns for ZnS nanoparticles synthesized in 0.2M concentration is shown in Fig 2. The X-ray pattern of ZnS nanoparticles shows sharper and stronger diffraction peaks at 25.879, 27.958, 31.449, 32.585, 33.324 and 33.324 units. These peaks correspond to cubic lattice structure of ZnS (Zinc blende) and assigned the planes (111), (220), (311). The different peaks were indicating high purity and well crystalline form ZnS. The presence of broad peaks in the XRD pattern implies presence of smaller particles. The d-spacing values are in good agreement with JCPDS No.77-2100.

Zinc blend and wurtzite are the two most popular structural configuration of ZnS. Due to size effect the peaks broaden and then widths become larger as the crystal becomes smaller. Ghosh et al [11] reported that the broadening of the peak may also occur due to micro strains of the crystal structure arising from defects like dislocation and twinning etc. There is a slight shift in the peak due to internal stress.

B. FTIR Analysis:

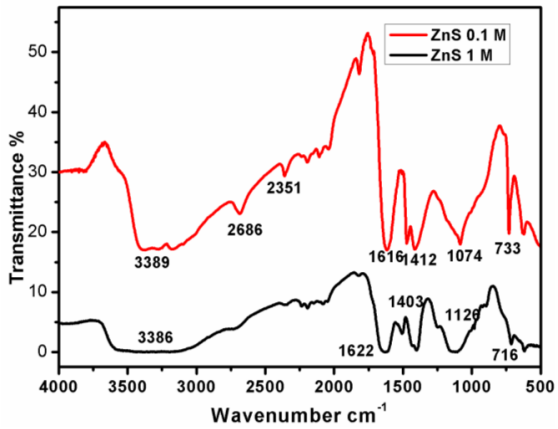

Fig 4. FTIR pattern for ZnS with 0.1M and 1M concentration

The FTIR spectrum of ZnS nanoparticles as shown in Fig 4 clearly indicates the characteristic functional groups which confirm the nanoscale properties of ZnS synthesized. The different peaks obtained at various points were compared with standard FTIR spectrum. Accordingly, the small peak observed at 3,448 cm-1 and corresponds to Hydrogen-bonded O-H stretch bending vibration of phenols and alcohol band; the set of small peaks present at 2,926 cm-1 and 2,856 cm-1 indicates the presence of C-H Stretch off C=O vibration of C-O and a small peak observed at 1,720 cm-1 represents C=O stretch correspond to Carboxylic acids band; a strong peak at 1,622 cm-1 represent C=O Stretch corresponds to Amide band; A small peak at 1,562 cm-1 represent N-H stretch corresponds to amide; a small peak observed at 1,543 cm-1 represent N-H bend is the characteristic of Amines-Secondary band; a small peak present at 1,517 cm-1 corresponds to N–O asymmetric stretch nitro compounds;

a small peak corresponds to 1,460 cm-1 and 1,421 cm-1 are C–H bend and alkanes bond respectively; a small peak observed at 1,398 cm-1 indicate N=O bend; a small peak observed at 1,369 cm-1 indicates C–H rock

alkanes; a broad peak observed at 9,16 cm-1 corresponds to O–H bend carboxylic acids. FTIR results of the present study on ZnS nanoparticles are in conformity with FTIR spectrum obtained by other research works for ZnS nanoparticles synthesized. Their spectrum indicates the presence of several strong peaks represents C-OH vibrations (1,088 cm-1 and 1,111 cm-1), O-H bending vibration (1,404 cm-1), O=C=O stretching (2,358 cm-1), phenol CO-H stretching (3,527 cm-1), N-H stretching (3,482 cm-1), alkenyl C-H stretch (3,010 cm-1) and amide N-H stretching (3,742 cm-1).

The peak at 405 cm−1 is the characteristic absorption of Zn–S bond. Other weak absorption peaks which corresponding to the sodium sulfate in the materials. This result show suitable agreement with previous works.

C. Microstructure of ZnS Nano Particles:

The Microstructure of the ZnS Nano particles were Analysed using Scanning Electron Microscope (ZEISS). The SEM images showed that the samples were composed of agglomerated and isolated particles and it reveals that small particles aggregate into secondary particles because of their extremely small dimension and high surface energy. Therefore, the diameter and the size distribution of the nanoparticles are difficult to be determined precisely by simply viewing the SEM images.

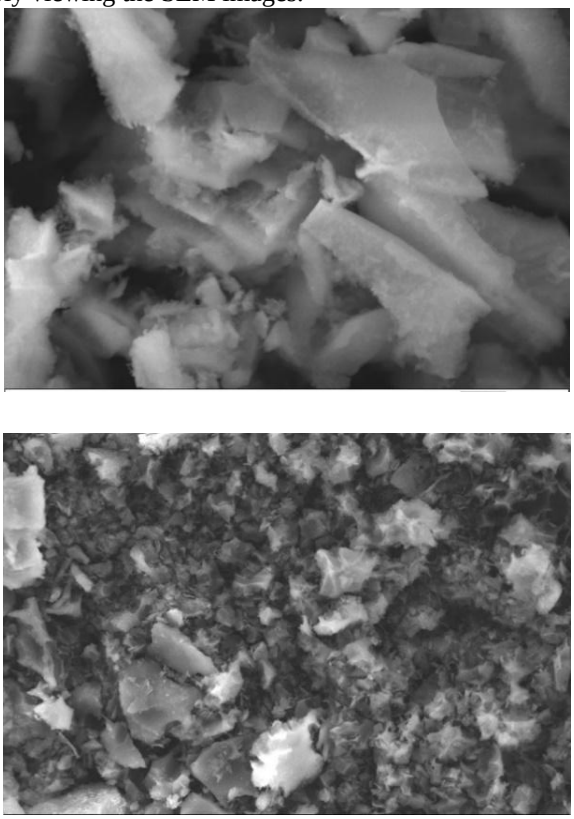

Fig 5: SEM structure of ZnS nanoparticles

D. Analysis from Ultra Violet – Visible Spectroscopy:

UV-Vis absorption spectra of various molar concentrations of ZnS materials were observed in SHIMADZU UV-1900 instrument with wavelength range from 200 to 900 nm. The solvent was diluted in deionized water. The maximum absorption peaks were observed at around 325 nm. The UV-Vis absorption spectra are shown in fig 6. UV-Visible spectra are a best supporting tool to identify and to recognize the optical absorption actions of semiconductor nanoparticles. The optical absorption spectrum of ZnS NPs is shown in fig 6. An absorption peak was observed in 325 nm for as synthesized ZnS nanoparticles and was in good agreement with the reported articles.

From the UV plot, the energy band gap is measured with the help of Tauc relation, The graph is plotted between (hv) vs $(\alpha h\nu)^2$

Where,

α = Absorption coefficient,

h = Plank constant (js)

A = Optical constant

ν = Frequency (Hz)

Eg= Energy band gap (eV)

From the tauc plot, the band gap of various concentration of ZnS materials were determined and the values are occurred in 3.1 eV to 3.6 eV.

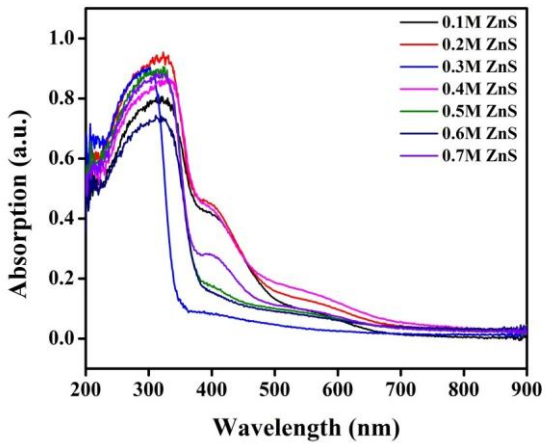

Fig. 6 UV-Vis absorption spectra of ZnS

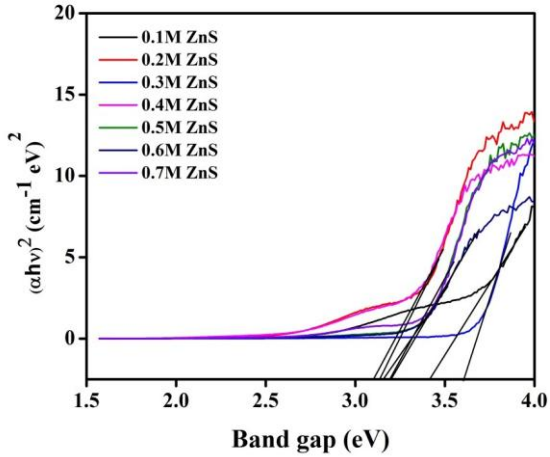

Fig.7: Band gap of ZnS

IV. PHOTOLUMINESCENCE

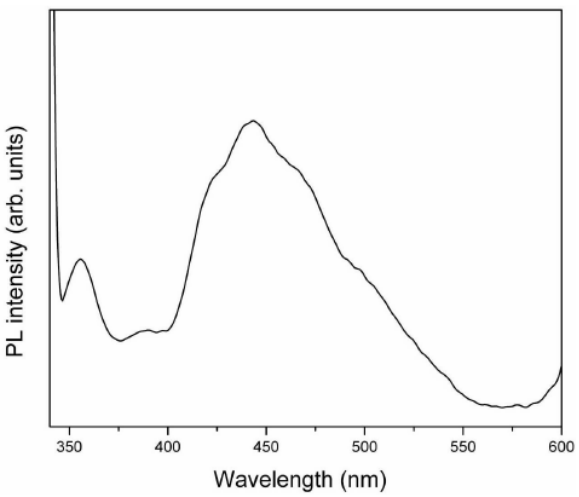

Fig 8: Photoluminescent spectrum of ZnS

The PL spectrum of the as-synthesized ZnS NPs is shown in fig 8. From the data it is evident that there is a strong emission band at about 448 nm and this could be due to the emission of blue fluorescence attributed to the recombination that has been taken place between the shallow electron trap states (i.e) S vacancy - the VB(valence band) and CB(conduction band) – Zn vacancy trap, respectively.

V. CONCLUSION

ZnS NPs were successfully synthesized by coprecipitation method. The calculated particle size from Debye-Scherrer formula was approximately 10 nm. The obtained structure well coincides with the JCPDS file and the structure is confirmed that Zinc Cube blended. A morphological study of SEM shows rock-like structure with agglomeration. The FTIR studies inferred the presence of stretching and bending assignments. The inference from UV absorption of 325 nm clearly indicates the blue shift. The investigation on photoluminescence evidenced that there is an emission at 448 nm. These results affirm that the synthesized material can be used in photovoltaic technology especially as a buffer layer in solar cells.

REFERENCES

1. Rui-Wei You, Yen-Pei Fu,, “Zinc Sulfide Buffer Layer for CIGS Solar Cells Prepared by Chemical Bath Deposition,” Adv. Technol. Innov, vol. 2(3), pp. 95 – 98, 2016.
2. P. Asha, M. Rajeswari and B. Bindhu, “Zinc sulfide nanoparticles: processing, properties and applications: an overview”, J Chem Pharm Sci, Vol.9(4), pp. 2047-2052, 2016.
3. Salim Oudah Mezan, Abdullah Hasan Jabbar, Maytham Qabel Hamzah, Alaa Nihad Tuama, Nabeel Naeem Hasan, Mohd Arif Agam, “Synthesis and Characterization of Zinc Sulphide (ZnS) Thin Film Nanoparticle for Optical Properties,” J. Glob. Pharm. Technol., vol. 10(07), pp. 369-373, 2018.
4. Mahdi H. Suhail, Omed Gh. Abdullah, Raoof A. Ahmed, Shujahadeen B. Aziz, “Photovoltaic Properties of Doped Zinc Sulfide/n-Si Heterojunction Thin Films”, Int. J. Electrochem. Sci., vol. 13, pp. 1472 – 1483, (2018).
5. V.B. Pujari, D.J. Dhage, and L.P. Deshmukh, Photo-voltaic Study of Hg Doped ZnS Thin Films, Inter. J. of Appl. Innov. Eng. Man., vol. 2(2), pp. 275, 2013.
6. E.U. Masumdar, L.P. Deshmukh, S.H. Mane, V.S. Karande, V.B. Pujari, and P.N. Bhosale, CdSe : Sb electrode for photoelectrochemical applications, J. Mater. Sci. Mater. Electron., vol. 14, pp.43, (2003).
7. S. Hossain, N. Amin, and T. Razykov, Prospects of back contacts with back surface fields in high efficiency ZnxCd1-xs /CdTe solar cells from numerical modeling, Chalcogenide Lett., vol.8, pp.187, (2011).
8. M.A. Akram, S. Javed, M. Islam, M. Mujahid, and A. Safdar, Arrays of CZTS sensitized ZnO/ZnS and ZnO/ZnSe core/shell nanorods for liquid junction nanowire solar cells, Sol. Energ. Mater. Sol. Cells, vol. 146,pp.121,(2016).
9. M. Guo, X. Zhu, and H. Li, Comparative study of Cu2ZnSnS4 thin film solar cells fabricated by direct current and pulse reverse co-electrodeposition, J. Alloy. Compd., vol. 657, pp.336, (2016).
10. C. Calderon, J.S. Oyola, P. Bartolo-Perez, and G. Gordillo, Studies in CuInS2 based solar cells, including ZnS and In2S3 buffer layers, Mater. Sci. Semicon. Proc., vol. 16, pp. 1382, (2013).
11. M.K.Ghosh, S.Anand, R.P.Das, Effect of dissolved impurities during ammonia leaching of pure zinc sulphide, Hydrometallurgy, Vol.22(1–2), pp.207-221, 1989.

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