CZTS A Pinnacle for the Solar Future

Mayank Sharma^{1*}, Vishal Bharti² and Anurag Vats²

¹Physics (Hons.), Motilal Nehru College, New Delhi - 110021, Delhi, India; anurag.16029@ggnindia.dronacharya.info ²Computer Science & Engineering, Dronacharya College of Engineering, Gurgaon - 123506, Haryana, India; mayanksharma123456789@gmail.com, hodcse@ggnindia.dronacharya.info

Abstract

Objectives: To study the characteristics of CZTS. **Methods/Statistical analysis**: Solvothermal method was employed for the preparation of CZTS. Various characterization techniques such as X-ray diffraction, UV-Vis Spectroscopy were used. **Findings**: Optical band gap, various peaks in X.R.D were calculated and the findings were in consensus with the existing data. **Application/Improvement:** CZTS holds a great aptness as a Photovoltaic material.

Keywords: Absorption Coefficient, Band Gap, Photovoltaic, Solvothermal

1. Introduction

The challenge of the present century is to create a technology or material that can make use of the some ever-lasting free energy resource so that all the humans can eat the fruits of such a technology for the rest of their lives. Solar energy is one such a resource. It's free, ever-lasting, and highly energetic. The sun delivers more energy to the earth in just one hour than is currently used worldwide in one year¹. But the problem is *"How to exploit such massive energy?"* CZTS is one potential answer.

2. CZTS

CZTS is a photovoltaic semiconducting material which converts the light (Photo) energy into electric (voltaic) energy. A material is typically said to be semi conducting if the band gap is less than 3 eV. In this particular material the band gap is around 1.4 eV-1.6 eV, which is considered ideal for photovoltaic applications. CZTS is a quaternary (comprising of four elements) P-type semiconductor compound^{2–6}. It is comprised of copper, zinc, tin and sulphide in a particular stoichiometric ratio and its chemical formula is Cu_2ZnSnS_4 . All the constituent elements of this semiconducting material are environment friendly and available in abundance in nature. It is a direct band gap

*Author for correspondence

material which nullifies the chances of energy losses in the form of heat radiations (Phonon).

2.1 Energy Band

The energy band diagram in Figure 1 depicts the valence and conduction band. The allowed energy levels are so near to that they, in a few cases, are considered as continuous which is reasonable approximation in some calculation but, it should always be retained in memory that the band is actually finite number of very closely spaced energy level.





2.2 Direct Band Gap

In direct band-gap material, the maximum energy level of the valence band aligns with the minimum energy level of the conduction band with respect to momentum. In this type, typically momentum and energy conservations are valid.

The pictorial representation of direct band gap is illustrated in Figure 2.



Figure 2. Energy-momentum space diagram.

3. Methods of Preparation

3.1 Solvothermal Method

It is a method of preparation of crystals which involves the use of non- aqueous solution in an autoclave with the aid of precursor. A precursor is a compound that participates in a chemical reaction in order to produce another compound.

A schemic diagram of solvothermal method has been depicted in Figure 3.



Schematics of electrochemical deposition of CZTS and a multi-bath electrodeposition-annealing approach

Figure 3. Solvothermal method.



Figure 4. (A)Electrochemical method (B) X- ray diffraction.

3.2 Electrochemical Deposition

Electrochemical deposition is a coating technique which involves reduction of cations in organic solution by supplying potential difference with external source of EMF as shown in Figure 4.

4. Basic Terminologies

4.1 Absorption Coefficient (α)

Absorption coefficient is an optical parameter which relates the lessening of intensity of light, once it is passed through a substance the thickness. It determines how far the light can penetrate into a particular material before being absorbed.

4.2 Solar Cell

It is a device that uses the photovoltaic technology to produce (or store) voltage and produce electricity from sunlight.

4.3 Thin Film Solar Cell

A solar cell that is built by deposition of one or multi-thin photovoltaic layers on substance such as glass or metal.

5. Characterization of CZTS

5.1 X-Ray Diffraction

X-Ray diffraction (XRD analysis) is a peculiar approach used in decisiveness of crystallinity of a compound. A technique which helps to study and identity the atomic and molecular structure of crystal in which crystalline atom cause a beam of incident X-Rays to diffract into many specific angular directions, predicted by Bragg's Law. Due to similar iso-electronic nature and similar structural properties of zinc and copper cat-ions, it is very difficult to differentiate between two crystals forms of CZTS: Kesterite and Stannite.

The XRD of CZTS is depicted in Figure 5.

5.2 Optical Characterization

UV-VIS SPECTROSCOPY: It gives the measurement of attenuation of beam of light after it passes through a sample or reflection from a sample surface which helps to check the purity of sample and various optical coefficients.



Figure 5. UV-vis spectroscopy.

Figure 6 shows characteristic plot of UV-VIS Spectroscopy.

Figure 6 also shows the plot to evaluate optical absorption coefficient.

The value of optimal band gap is 1.5 eV(approx.)^{7.8}

The absorption coefficient (a) is of the order of 10^4 cm⁻¹ ($^{-1}$ cm⁻¹) cm⁻¹ ($^{-1}$ cm⁻¹ ($^{-1}$ cm⁻¹ ($^{-1}$ cm⁻¹) cm⁻¹ ($^{-1}$ cm⁻¹ ($^{-$



Figure 6. The plot of $(\alpha h\nu)$ ^2versus hv, where α is the optical absorption coefficient, and h ν is the energy associated with single incident photon. The optical band gap (Eg) is calculated.

6. Discussion

There are various methods for characterization of CZTS each for its specific purpose. For instance, Raman Spectroscopy is used to study and identify various molecules by carefully investigating molecule vibrations. Scanning Electron Microscopy is used to obtain information about surface topology and composition. The electron in the beam interact with the sample to produce various signals.

Transmission Electron Microscopy is used to study the internal composition of the material under investigation, etc. A lot of people in the scientific community are currently working on this exciting photovoltaic aspect and a lot of papers on the preparation, characterization, ligand substitution in CZTS have been published. Various types of studies such as Photo electrochemical studies at various places around the globe have been and are still being carried out to explore more and more about it.

The highest efficiency obtained for CZTS solar cell (0.42 cm^2) till date is **12.6%** ^{12–14}.

7. Acknowledgement

The Project was funded by Department of Physics, IISC Bangalore. The project could not have been completed without the help of the funding and the priceless advice from my mentor.

8. Conclusion

CZTS is an aspiring bargain in thin film solar cells due to its superior material properties. For instance, its band gap of energy valued between 1.4 eV-1.6 eV which makes it highly efficient, splendidly backed up by large coefficient of absorption 10⁴ cm⁻¹. The composition of CZTS involves more abundant Zn and Sn, making it a better choice than the other material in its league for low cost solar cell. Its preparation involves less harmful, eco-friendly and less toxic when it is compared to other solar cells like CIGS.

9. References

- Environment sunlight striking earth's surface in just one hour delivers enough energy to power the world economy for an entire year [Internet]. [cited 2015 Jun 17]. Available from: http://www.alternet.org/environment/ sunlight-striking-earths-surface-just-one-hour-deliversenough-energy-power-world.
- Lokhande CD, Pawar SH. Electrochemical photovoltaic cells for solar energy conversion. Materials Chemistry and Physics. 1984; 11(3):201–77. Crossref
- 3. ScreggJ, Dale P, Peter L, Zopp G, Forbes L. Physicastatus solidi. 2008, 245, pp. 1772. Crossref
- Riha S, Fredrick S, Sambur J, Liu Y, Prieto A, Parkinson B. Photoelectrochemical characterization of nanocrystalline thin-film Cu2ZnSnS4 photocathodes. Applied Materialsinterfaces. 2011; 3(1):58–66. Crossref
- Zhang X, Shi X, Ye W, Ma C, Wang C. Electrochemical deposition of quaternary Cu2ZnSnS4 thin films as potential solar cell material. Applied Physics. 2009; 94(2):381–6.

- Jimbo KK, Kimura R, Kamimura T, Yamada S, Maw W, Araki H, Oishi K, Katagiri H. Thin Solid Films. 2007, 515, pp. 5997. Crossref
- 7. Pawar SM, Moholkar AV, Kim IK, Shin SW, Moon JH, Rhee JJ, Kim JH. Current Applied Physics. 2010; 10:565. Crossref
- 8. Thin Film solar cell [Internet]. [cited 2017 Mar 22]. Available from: http://en.wikipedia.org/wiki/Thin-film_ solar_cell.
- Solar Froniter [Internet]. [cited 2013 Dec 10]. Available from: http://www.solar-frontier.com/eng/news/2013/ C026764.html.
- Ito K, Nakazawa T. Jpn. J. Appl. Phys. 1998; 27(1998):2094. Crossref
- 11. Tanaka T, Nagatomo T, Kawasaki D, Nishio M, Guo Q, Wakahara A, Yoshida A, Ogawa H. Journal of Physics Chem. Solid 2005; 66:1978. Crossref