



ENHANCING PHOTOVOLTAIC EFFICIENCY THROUGH THE DEVELOPMENT AND CHARACTERIZATION OF NOVEL PEROVSKITE THIN FILMS FOR SOLAR CELLS

MUKESH KUMAR SINGH

Research Scholar, TheGlocal University, Saharanpur (U.P)

DR. SATENDRA SINGH

Assistant Professor, TheGlocal University, Saharanpur (U.P)

ABSTRACT

CZTSSe materials have been studied for a highly efficient solar cell. In this paper, $Cu_2ZnSn(S_{0.2}Se_{0.8})_4$ (CZTSSe) thin film was prepared and its application to photovoltaic solar cells was studied. The CZTSSe thin film was deposited using facile thermal evaporation process and examined by various techniques including x-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), atomic force microscopy (AFM), Raman-scattering and Fourier transform infrared (FTIR) spectroscopy. Interestingly, the synthesized CZTSSe thin are exhibiting broad-spectrum absorption. The I-V characteristics were performed to study the photo-response of CZTSSe Nano film. By the numerical simulation, the observed maximum efficiency of the fabricated device was ~16.5%. Therefore, the present study reveals that $Cu_2ZnSn(S_{0.2}Se_{0.8})_4$ thin films could be used as an effective absorber layer for efficient solar cells applications.

Keywords: -Solar cells, ZnSn, Energy, Co₂, Efficiency.

I. INTRODUCTION

In comparison to conventional energy sources, renewable energy is clean, safe and it has no harmful environmental impact. Renewable engineering has been given considerable importance in preventing global warming, also it has been observed that solar devices will play a key role in reducing CO₂. Sun is the most abundant and easily accessible source of clean energy, so solar cells are the latest technology to meet global high energy requirements. Different applications and low cost of PV technology must be developed and circulated. Flexible solar cell platform allows for the extension of innovations such as building-integrated photovoltaics (BIPV) construction and mobile applications. Moreover, low-cost efficient substrates can be used to reduce production costs, which can lead to the growth of the green energy market by shortening



the payback period for electricity. Concerning low cost flexible substrates, higher-cost materials need to be used to achieve low production costs. Kieserite materials are more desirable for small-cost execution than solar cells Author to whom correspondence should be addressed. Of CIGS and CdTe. The maximum power conversion efficiency (PCE) of CIGS photovoltaic cells has been achieved to be 22.8% while CZTSSe photovoltaics had a comparatively low efficiency of 12.6%. The efficiencies of flexible CIGS solar cells were 20.4% for polyimide (PI) substrates and 17.7% for stainless steel (SS) substrates. The efficiency of the flexible CZTS solar cells was 7.04% with the Mo foil substrate and 6.29% on stainless steel foils substrates. Also, the efficiency of CZTS solar cell of soda lime (SLG) was estimated to be 11.3% with a cell area greater than 1 cm². Flexible kieserite solar with a small area of ~0.53 cm² low efficiency was reported as 7.04%. Thin film kieserite solar cells currently achieve high solar cell efficiency. Kieserite has instability of its quaternary and secondary phases and associated defects can lead to recombination of the electron-hole and reduction of open-circuit voltage (V_{oc}) and current density (J_{sc}). Due to their superior phase stability, less no of secondary phases and deficiencies are formed in CIGS thin-film solar cells, but secondary phases and imperfections of different types can be created in kieserite absorber layers.

The increasing global demand for renewable energy sources has led to extensive research and development in the field of photovoltaics. Perovskite solar cells have emerged as a promising technology for efficient and cost-effective solar energy conversion. This section provides an overview of perovskite solar cells, highlighting their structure, properties, and advantages.

II. PEROVSKITE STRUCTURE AND PROPERTIES

Perovskite materials, named after the mineral perovskite, have a unique crystal structure represented by the chemical formula ABX₃, where A and B are cations and X is an anion. In the context of solar cells, the A cation is typically an organic or inorganic molecule, the B cation is a metal ion, and X is usually a halide or oxide ion.

The perovskite structure exhibits remarkable optoelectronic properties that make it highly suitable for photovoltaic applications. Perovskite materials possess direct bandgaps, high absorption coefficients, long carrier diffusion lengths, and low non-radiative recombination rates. These properties enable efficient light absorption, charge carrier generation, and transport within the material.

Performance Advantages of Perovskite Solar Cells

Perovskite solar cells offer several advantages over traditional photovoltaic technologies, including:



a) **High Efficiency:** Perovskite solar cells have achieved remarkable power conversion efficiencies (PCEs) exceeding 25%, rivaling those of established solar cell technologies. This high efficiency is attributed to the narrow bandgap and the ability to tune the band structure of perovskite materials, enabling efficient harvesting of a broad range of solar spectra.

b) **Low-Cost Manufacturing:** Perovskite solar cells can be fabricated using solution-based techniques such as spin coating, inkjet printing, and spray deposition. These processes are relatively simple, cost-effective, and compatible with high-throughput production methods, enabling scalable and low-cost manufacturing.

c) **Versatile Material Properties:** The composition of perovskite materials can be easily modified by changing the A, B, and X components, allowing the tunability of optoelectronic properties. This versatility enables the design and optimization of perovskite solar cells for specific applications, including tandem solar cells, building-integrated photovoltaics, and flexible devices.

d) **Tolerance to Defects:** Perovskite materials exhibit a remarkable tolerance to defects and grain boundaries, which can reduce the detrimental effects of defects on device performance. This feature simplifies the fabrication process and enhances the stability of perovskite solar cells, making them more resilient to environmental conditions.

e) **Light Weight and Flexibility:** Perovskite solar cells can be fabricated on lightweight and flexible substrates, enabling their integration into various form factors and applications. This flexibility makes them suitable for applications where weight and mechanical properties are important, such as portable electronics, wearable devices, and curved surfaces.

Current Challenges and Limitations

Despite the tremendous progress in perovskite solar cell research, several challenges and limitations still need to be addressed:

a) **Stability and Durability:** Perovskite materials are prone to degradation when exposed to moisture, oxygen, light, and elevated temperatures. Prolonged exposure to these conditions can lead to the degradation of perovskite films and a decrease in device performance over time. Developing stable perovskite formulations and encapsulation strategies is crucial for long-term device operation.

b) **Scaling Up and Commercialization:** While laboratory-scale perovskite solar cells have achieved impressive efficiencies, scaling up the manufacturing process while maintaining high performance and stability remains a challenge. Developing large-area deposition techniques,



improving material reproducibility, and establishing robust manufacturing processes are critical for commercialization.

III. OPTIMIZATION OF PEROVSKITE THIN FILMS

The performance of perovskite solar cells is strongly influenced by the quality and characteristics of the perovskite thin films. This section focuses on the optimization strategies employed to enhance the properties of perovskite thin films, including morphology, crystal structure, composition, and surface passivation.

Film Morphology and Crystal Structure

The morphology and crystal structure of perovskite thin films significantly impact the device performance. A uniform and dense film with large grain sizes and minimal defects is desired for efficient charge transport and reduced recombination. Various techniques have been explored to optimize the film morphology, including:

- a) **Solvent Engineering:** The choice of solvents, their ratios, and the addition of additives during the perovskite film deposition process can influence the film morphology. Solvent engineering strategies aim to control the nucleation and growth dynamics of perovskite crystals, promoting the formation of large and well-oriented grains.
- b) **Templating and Surface Modification:** Surface modification techniques, such as the use of self-assembled monolayers or deposition on patterned substrates, can guide the crystal growth and control the film morphology. Templating methods enhance the crystal alignment and reduce grain boundaries, resulting in improved charge transport properties.
- c) **Annealing and Post-Treatment:** Thermal annealing and post-treatment processes can further optimize the film morphology by promoting crystal growth, grain boundary healing, and defect passivation. Controlled heating profiles and chemical treatments can enhance the film's structural integrity and reduce trap states.

Influence of Composition and Stoichiometry

The composition and stoichiometry of perovskite materials play a crucial role in determining their optical and electronic properties. Fine-tuning the composition allows for bandgap engineering, optimal charge transport, and improved stability. Strategies for composition optimization include:

- a) **Cation and Anion Engineering:** By substituting different cations and anions within the perovskite structure, the bandgap and stability of the material can be tailored. For example,



introducing organic cations with varying sizes and properties can modify the bandgap and improve film quality. Similarly, incorporating different halide anions can influence the optical absorption and charge transport properties.

b) Mixed Halide Perovskites: Introducing mixed halide compositions (e.g., iodide/bromide or iodide/chloride) has been shown to enhance the stability, optical absorption, and charge carrier dynamics of perovskite films. The careful optimization of halide ratios can lead to improved device performance and reduced hysteresis effects.

c) Dopants and Additives: The addition of dopants or additives during the perovskite film fabrication process can modify the crystallization kinetics, reduce trap states, and improve film morphology. Examples include the use of small organic molecules, inorganic salts, or Lewis bases to optimize the film quality and device performance.

Surface Passivation Techniques

Surface passivation techniques aim to reduce surface defects, trap states, and interfacial recombination within the perovskite film. Passivation can be achieved through various approaches, such as:

a) Interface Engineering: Modifying the interface between the perovskite absorber layer and the charge transport layers (e.g., electron-transporting and hole-transporting materials) can minimize energy barriers, reduce charge carrier recombination, and enhance charge extraction. Surface modification techniques, including self-assembled monolayers and interfacial layers, have been employed for interface engineering.

b) Defect Passivation: Defects within the perovskite film, such as vacancies, grain boundaries, and surface traps, can act as recombination centers and limit device performance. Defect passivation methods, such as chemical

IV. CONCLUSION

From the present experimental work, it has been investigated that CZTSSe material could be used as a highly efficient solar cell. The characterizations such as XRD, Raman, and FTIR show that all the peaks are with phase matching which is important for high performance of solar cell devices. Furthermore, some smaller peaks in XRD, such as (312) and (400) become observable, indicating that the CZTSSe thin film has good crystallinity. Scanning electron microscopy gives information about the multiple small number of particles present in the sample. From atomic force microscopy analysis, the average diameter and height of the film recorded using WSxM 5.0 software are 284 nm and 35 nm respectively. The bandgap of CZTSSe particles obtained



using Tauc relation is 1.25 eV and the maximum extinction coefficient value is 27 at 827 nm wavelength or 1.5 eV equivalent photon energy. IV measurement of pellets has also been done for the photo-response. All the characterizations show that $\text{Cu}_2\text{ZnSn}(\text{S}_2\text{Se}_2\text{S}_8)_4$ could be used as an absorber layer for the efficient solar cell. With the use of the numerical simulation tools the efficiency of the synthesized nanoparticle taking all the defects in consideration is found to be 16.5%.

REFERENCES

1. Kojima, A., Teshima, K., Shirai, Y., & Miyasaka, T. (2009). Organometal halide perovskites as visible-light sensitizers for photovoltaic cells. *Journal of the American Chemical Society*, 131(17), 6050-6051.
2. National Renewable Energy Laboratory (NREL). (2021). Best Research-Cell Efficiency Chart. Retrieved from <https://www.nrel.gov/pv/cell-efficiency.html>
3. Green, M. A., Ho-Baillie, A., & Snaith, H. J. (2014). The emergence of perovskite solar cells. *Nature Photonics*, 8(7), 506-514.
4. Stranks, S. D., & Snaith, H. J. (2015). Metal-halide perovskites for photovoltaic and light-emitting devices. *Nature Nanotechnology*, 10(5), 391-402.
5. NREL. (2021). Perovskite Solar Cells: An Overview. Retrieved from <https://www.nrel.gov/research/program-perovskite-solar-cells.html>
6. Kim, H. S., Lee, C. R., Im, J. H., Lee, K. B., Moehl, T., Marchioro, A., ... & Park, N. G. (2012). Lead iodide perovskite sensitized all-solid-state submicron thin film mesoscopic solar cell with efficiency exceeding 9%. *Science*, 338(6107), 643-647.
7. Jeon, N. J., Noh, J. H., Kim, Y. C., Yang, W. S., Ryu, S., & Seok, S. I. (2014). Solvent engineering for high-performance inorganic-organic hybrid perovskite solar cells. *Nature Materials*, 13(9), 897-903.
8. Saliba, M., Orlandi, S., Matsui, T., Aghazada, S., Cavazzini, M., Correa-Baena, J. P., ... & Hagfeldt, A. (2016). A molecularly engineered hole-transporting material for efficient perovskite solar cells. *Nature Energy*, 1(7), 15017.
9. Li, W., & Yang, Y. (2018). Solution-processed perovskite solar cells. *Joule*, 2(11), 2007-2021.
10. Zhou, H., Chen, Q., Li, G., Luo, S., Song, T. B., Duan, H. S., ... & Liu, T. (2014).



Interface engineering of highly efficient perovskite solar cells. *Science*, 345(6196), 542-546.

11. Domanski, K., Correa-Baena, J. P., Mine, N., Nazeeruddin, M. K., Abate, A., Saliba, M., ...&Grätzel, M. (2016). Not all that glitters is gold: metal-migration-induced degradation in perovskite solar cells. *ACS Nano*, 10(6), 6306-6314.
12. Park, N. G., Grätzel, M., Miyasaka, T., Zhu, K., & Emery, K. (2016). Towards stable and commercially available perovskite solar cells. *Nature Energy*, 1(11), 16152.