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Optimization of hole transport layers for Cu_2FeSnS_4 solar cells via SCAPS-1D simulation: Investigating the impact of interface defects on practical efficiency limits

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ABSTRACT

The quaternary Cu_2FeSnS_4 (CFTS) chalcogenide garners significant interest as a sustainable alternative in solar cell applications due to its abundant and non-toxic composition. This study uses SCAPS-1D simulations to examine the performance of CFTS solar cells (ITO/HTL/CFTS (400 nm)/CdS (200 nm)/ZnO (10 nm)/Al) using three distinct hole transport layers (HTLs), namely NiO_x, Cu_2O, and CuI. The simulations led to a deeper understanding of their practical efficiency limits, considering the huge gap in the theoretical and experimental efficiency values reported earlier. The investigations reveal the precise mechanisms and the influence of hole transport layers on the device performance, specifically the bulk and interface defect densities. In addition, the other major aspects of CFTS solar cell performance, including the correlation between electric field, generation rate, and recombination rate are discussed. Our observations suggest that while identifying a suitable hole transport layer, it is imperative to consider these parameters, which are often overlooked in many numerical simulations, resulting in unrealistic theoretical efficiency values in contrast to the low efficiency observed in practical devices. Here, the optimized ITO/CuI/CFTS/CdS/ZnO/Al configuration demonstrated a maximum efficiency of 5.05 %, with a V_{oc} of 0.55 V, J_{sc} of 14.5 mA/cm^2, and FF of 61.8 %, which are in accordance with experimental values reported. Thus, the study here emphasizes the importance of considering the defect densities, electric field, generation rate, and recombination rate to bridge the gap between theoretical and practical efficiency values, which can significantly influence the design strategies to enhance the CFTS solar cell efficiency.

1. Introduction

The increasing global energy demands and the necessity of sustainable solutions drive the research in photovoltaic technology to achieve higher efficiency in low-cost devices fabricated using non-toxic materials. Over the past decade, quaternary chalcogenide materials, particularly kesterite-type, have garnered considerable attention due to their promising characteristics, including extrinsic p-type properties with an optimal band gap (1.2–1.8 eV), high absorption coefficients (1×10^{-4} cm^{-1}), and eco-friendly composition [1]. On the other hand, traditional quaternary materials such as CIGS, CdTe, and GaAs have also been prominent in thin-film photovoltaic technologies [2–5]. However, the transition to kesterite-type solar cells has been caused by the scarcity of Indium and Gallium, the limited availability of tellurium, and the toxicity of Cadmium.

1.1. Kesterite-type solar cells

Kesterite model solar cells, particularly CZTS solar cells, have demonstrated significant advancements, although their maximum efficiency remains relatively low, reaching approximately 15 %. Despite the potential for efficiencies up to 30 % according to the Shockley-Queisser limit, achieving such high efficiencies remains a challenge [6]. Copper-based chalcogenide has shown significant potential as a superior alternative to carbon-based renewable energy sources. Chalcogenide Cu_2FeSnS_4 (CFTS), which is composed of copper, iron, tin, and sulfur, has attracted interest for photovoltaic applications because of its energy band gap between 1.2 and 1.6 eV and an optical coefficient over 10^4 cm^{-1} [7–11]. The most widely used crystal structure of CFTS is tetragonal stannite, with I-42m space group, with a = b = 5.46 Å and c = 10.72 Å represented in Fig. 1. Among these quaternary materials, CFTS

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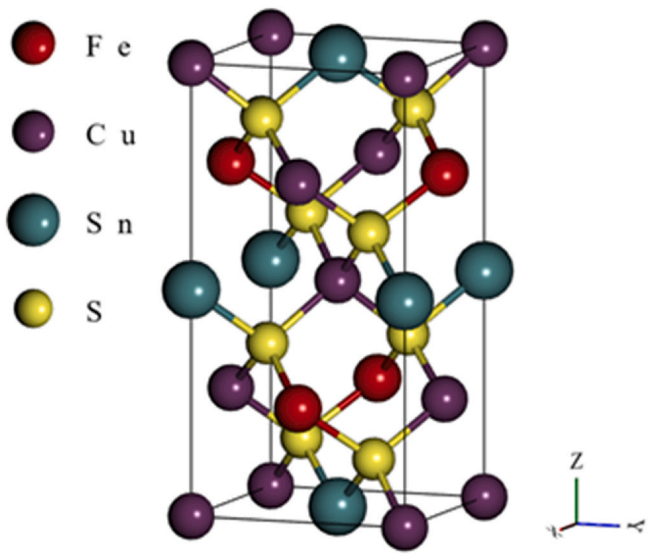

Fig. 1. Stannite structure of Cu_2FeSnS_4.

has emerged as a versatile material with applications ranging from solar cells to photo-electrodes in DSSCs [7,12–15], memory switching [16], and more [10,11,17,18]. Various numerical studies on CFTS solar cells have explained the device's performance based on different device parameters [19–23]. The highest reported efficiency for a CFTS solar cell is 2.9 % which has a device structure of ITO/Cu@-NiO/CFTS/Bi_2S_3/ZnO/Al fabricated through a solution-based process [13]. Here, Cu-doped NiO played a key role as the hole transport layer, while ZnO acted as an electron transport layer. The success of this design may be due to the unique electrical and structural properties of Cu as a dopant, which improved the integration of the hole transport layer, paving the way for further advancements in CFTS solar cell technology. The study's primary goal is to better understand the impact of hole transport layers and improve the CFTS solar cell efficiency while considering practical limitations.

The carrier lifetime, measured in seconds (τ), denotes the average time required for a minority carrier to recombine, which significantly influences the performance of photovoltaic cells. In the fabrication of photovoltaic cells, the minority carrier lifetime stands as a crucial parameter for solar cell characterization. It is intricately linked to the recombination rate, expressed as

$$\tau = \frac{\triangle n}{R} \tag{1}$$

Where 'τ' represents the minority carrier lifetime, 'R' signifies the recombination rate, and 'Δ' denotes the excess minority carrier concentration.

1.2. Hole transport layers in kesterite solar cells

Proper selection of the hole transport layer (HTL) can mitigate the rollover effect, lower the barrier height of the back contact, and minimize recombination losses of minority carriers at the back contact [24,25]. The primary role of HTL is to extract holes from the absorber layer and transfer them to the appropriate electrodes, so it is critical to comprehend the practical implications of selecting hole transport layers. Nickel oxide (NiO_x) materials are frequently used in perovskite-based devices, CdTe, and organic solar cells due to their p-type characteristics, high transmittance, and wide band gap of 3.5–3.9 eV. Their band structure aligns well with band edge levels of CZTS/CZTSe-type materials, minimizing recombination losses and enhancing charge carrier separation and transport which results in better open-circuit voltage and overall power conversion efficiencies. Besides, NiO_x offers advantages such as high conductivity, chemical stability, flexibility, high storage capacity, and low cost [26–30]. Similarly, cost-effective and eco-friendly Cu_2O exhibits high hole mobility and good band alignment for p-type quaternary chalcogenide absorber layers such as CZTS. The performance of oxide thin films can be enhanced by employing suitable deposition techniques. Incorporating oxide buffer layers such as Cu_2O and NiO_x reduces carrier recombination and serves as an efficient electron-blocking layers by introducing an intermediate energy band that promotes hole extraction and transport. Furthermore, the chemical stability of these oxides helps protect the underlying CFTS layer from oxidation. These are more resilient to environmental deterioration than organic buffer layers. NiO_x and Cu_2O have been deposited using sputtering methods, especially as it is used as the hole transport layers for chalcogenide solar cells, organic solar cells, as well as perovskite solar cells [29–32]. Numerous reports describe the utilization of RF and DC sputtering to produce thin films using NiO_x and Cu_2O, which will provide good adhesion and allow for appropriate tuning [33]. Oxide thin films are deposited by regulating the development conditions by maximizing appropriate variables such as oxygen partial pressures, temperatures, and deposition rates.

Their suitable valence band position, which aligns well with the CZTS layer reduces the energy barrier, facilitating effective hole extraction and lower interface recombination to yield enhanced power conversion efficiency [34]. This alignment enhances photovoltaic performance by minimizing energy and recombination losses at interfaces. Similarly, the cheap and non-toxic p-type CuI semiconductor has a larger band gap of 3.1 eV, offering excellent optical transmittance of 86 %, low cost, eco-friendliness, low extinction coefficient, and high hole mobility (0.5–2 $cm^2/V\cdot s$) [26,34–36]. Importantly, it has an ideal band alignment with the CZTS absorber layer [34] for the fabrication of the CFTS solar cells. CuI is deposited via thermal evaporation, a technique that, when conducted under vacuum conditions, minimizes the risk of oxidation. This method enhances the adhesion of CuI to glass substrates, and subsequent post-annealing further mitigates defect formation and improves the stability of the CuI thin films. CuI has been used as a hole transport layer in kesterite solar cells as well as perovskite solar cells, which improved the performance of photovoltaic devices [31,37–40].

Therefore, in this study, NiO_x, CuI, and Cu_2O were selected as suitable HTL materials to investigate their impact on the performance of CFTS solar cells, as they are composed of non-toxic elements and encompass both oxide and non-oxide materials. This study aims to enhance the efficiency of CFTS solar cells by incorporating suitable HTL and addressing fabrication challenges. In particular, surface passivation and surface imperfections due to material composition, and the presence of impurities, which also show deviation from the stoichiometry of CFTS, deposition temperature, as well as humidity, affect the fabrication process, which deteriorates the performance of CFTS solar cells. This detailed analysis ensures that potential defects and their impacts on device performance are accounted for, providing a realistic assessment of the solar cell's efficiency and reliability. The SCAPS-1D simulation framework relies on several simplifying assumptions, notably that all absorber layers are laterally homogeneous and free of structural defects. It does not account for lateral carrier transport or material inhomogeneities. Conductive secondary phases like Cu_2S, which could create shunting paths due to their unique electronic characteristics, are excluded from the model [41,42]. Instead, it assumes a uniform single-phase material with no representation of secondary phase geometry or interfacial effects. Defect states are considered to be evenly distributed throughout each layer, and interfaces are idealized, lacking interdiffusion, secondary phase formation, or potential drops caused by grain boundaries or conductive inclusions.

Similar efforts in CZTS-based solar cells have shown performance improvements [34,35], prompting further investigation into the impact of HTL on CFTS-based solar cells and their potential to increase efficiency using numerical simulations [35].

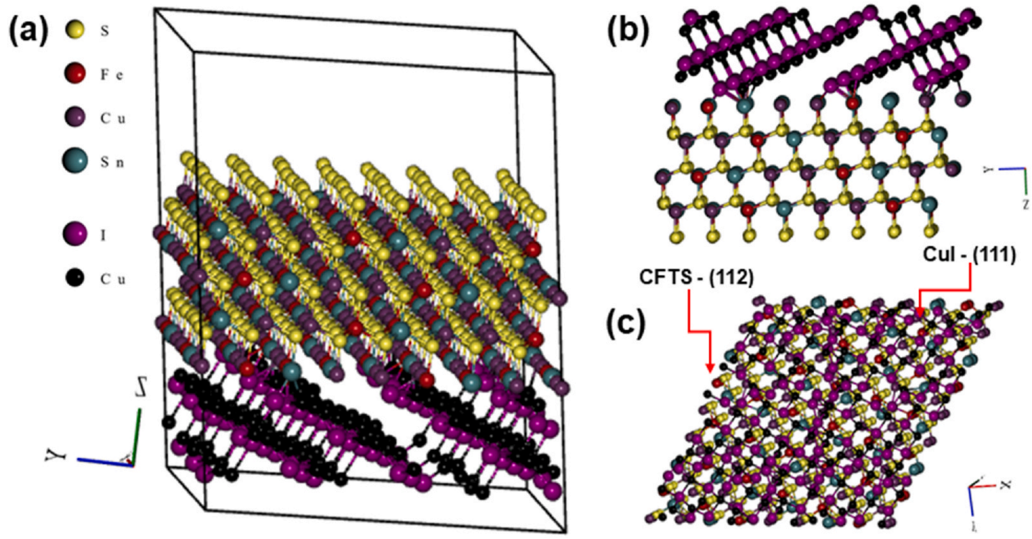

Fig. 12. CFTS/CuI Interface structure.

Table 9
Lattice mismatch of HTL/CFTS Interface.

HTL/CFTS Interface	Lattice parameters of HTL(Å)	Lattice mismatch (%)
CuI/CFTS	a = b = c = 6.05 [103]	9.06
NiO_x/CFTS	a = b = c = 4.17 [104]	25
Cu_2O/CFTS	a = b = c = 4.27 [105]	23

maximum efficiency was determined to be 50 nm with interface defect concentrations of 1×10^{10} cm^{-2} and shallow acceptor densities of 1×10^{18} cm^{-3}. The findings provide useful direction for further research and practical applications, emphasizing the need for precise material and structural changes to achieve optimum solar cell performance. The results highlight the necessity of HTL and structural modifications to attain maximum solar cell efficiency and offer helpful guidance for future research and real-world applications.

CRediT authorship contribution statement

M.K. Jyolsna Raj: Writing – review & editing, Writing – original draft, Validation, Software, Methodology, Investigation, Formal analysis, Conceptualization. **Kallol Mohanta:** Writing – review & editing, Validation, Supervision, Methodology, Investigation, Formal analysis. **Sebin Devasia:** Writing – review & editing, Validation, Supervision, Investigation, Formal analysis. **B. Geetha Priyadarshini:** Writing – review & editing, Validation, Supervision, Methodology, Investigation, Formal analysis, Conceptualization.

Data availability statement

The data that supports the findings of this study are available from the corresponding author upon reasonable request.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jpcs.2025.113193.

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