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Graded band-gap engineering for increased efficiency in CZTS solar cells

H. Ferhati [a], F. Djeffal [a, b, *]

[a] LEA, Department of Electronics, University Mostefa Benboulaid-Batna 2, Batna 05000, Algeria
[b] LEPCM, University of Batna 1, Batna 05000, Algeria

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ABSTRACT

In this paper, we propose a potential high efficiency $Cu_2ZnSn(S,Se)_4/CdS$ (*CZTS*) solar cell design based on graded band-gap engineering that can offer the benefits of improved absorption behavior and reduced recombination effects. Moreover, a new hybrid approach based on analytical modeling and Particle Swarm Optimization (*PSO*) is proposed to determinate the optimal band-gap profile of the amended *CZTS* absorber layer to achieve further efficiency enhancement. It is found that the proposed design exhibits superior performance, where a high efficiency of *16.9%* is recorded for the optimized solar cell with a relative improvement of *92%*, compared with the reference cell efficiency of 8.8%. Likewise, the optimized *CZTS* solar cell with a graded band-gap enables achieving a higher open circuit voltage of *889 mV*, a short-circuit current of *28.5 mA* and a fill factor of *66%*. Therefore, the optimized *CZTS*-based solar cell with graded-band gap paradigm pinpoints a new path toward recording high-efficiency thin-film solar cells through enhancing carrier collection and reducing the recombination rate.

1. Introduction

In today's energy production, the deployment of photovoltaic systems with larger affordability is expected to be an economically advantageous technique for providing carbon neutral clean energy [1]. Despite this, it seems to be of great significance to enhance the solar cell performance and reduce the fabrication cost of photovoltaic panels [1,2]. The c-*Si*-based technology provides higher efficiency value of *26.6%*, while it exhibits several problems mainly associated with the high manufacturing cost that arises from the purification, crystallization, and processing steps [2,3]. Otherwise, cost-effective technologies based on organic/inorganic, perovskite, and dye-sensitized designs still suffer from the low conversion efficiency and reliability [3–5]. Alternatively, thin-film chalcogenide $CuIn_xGa_{(1-x)}Se_2$ (*CGIS*) solar cell has attracted certainty a great interest due to its high stability as well as its superior efficiency value of *22%* [5–7]. However, the use of rare metals or toxic materials like: gallium, germanium, indium and cadmium for the *CGIS*-based solar cells can prevent achieving high efficiency/cost ratio. In this regard, for the continuous progress of the thin-film solar cells, kesterite *CZTS* material is believed to be a substitutional earth-abundant, inexpensive and nontoxic material with distinctive optical properties [8–10]. In fact, this material exhibits a high absorption coefficient ($>10^4 cm^{-1}$) and enables the opportunity for adjusting band-gap appropriately [11]. To this extent, following the DFT calculations *CZTS* is considered naturally as an important chalcogenide *p*-type semiconducting material having a direct optical tunable band-gap of *1.52 eV*, which makes it suitable for optoelectronic applications [11–13]. These advantages make it as a potential candidate to overcome the trade-off between both high-efficiency and low fabrication cost. For this purpose, a great deal of attention has been paid to *CZTS*-based technology in order to improve the solar cell performance, where *9.5%* efficiency for the conventional *CZTS* structure, *12.6%* for *Se*-alloying kesterite-based design, and *11.2%* for *CZCTS* solar cell with *Cd*-containing have been recorded [8–11]. However, the *CZTS*-based solar cell power efficiency is considered still far from that offered by *CIGS*-thin film solar cell (*22%*) [13,14]. This is mainly due to the extensive limitations typically observed for kesterite solar cells, which are associated with the short minority carrier lifetime and the high series resistance imposed by the contact barrier due to the formation of the MoS_2 at the *CZTS/Mo* interface [15–17]. In this context, several published works are focused on addressing these

* Corresponding author. LEA, Department of Electronics, University Mostefa Benboulaid-Batna 2, Batna 05000, Algeria.
E-mail addresses: faycal.djeffal@univ-batna.dz, faycaldzdz@hotmail.com (F. Djeffal).

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problems in order to reach high-efficiency *CZTS* solar cells by proposing new designs based on rear passivation layers, *In/Cd* hybrid buffers and *CZTS/*CeO_2 solar cell design [10–17]. Yet, the incapability to avoid the high series resistance and the recombination effects, which are mainly depending on the carrier lifetime, still persist and prevent achieving competitive efficiencies. Consequently, new alternative approaches should be developed to overcome the above mentioned problems in order to achieve high-performance photovoltaic devices. In this context, the use of the graded band-gap aspect can be beneficial for improving the solar cell performance. In other words, increasing linearly the *CZTS* band-gap through varying the *Se* content can be a substantial solution to modulate the electric field in the absorber layer and enhance the transport mechanism of the photogenerated carriers [18]. To the best of our knowledge, no investigations based on combining both graded band-gap engineering and global optimization technique were proposed to boost and maximize the power efficiency in *CZTS* solar cells. For this purpose, we present in this paper, a new hybrid approach based on analytical modeling of the proposed design including the impact of the graded band-gap profile, combined with *PSO*-based metaheuristic computation. The merit of this approach is to determinate the global optimized graded band-gap profile to avoid the recombination effects and enhance the solar cell absorption behavior. The obtained results make the optimized design potential alternative for avoiding the recombination losses and increasing the optical absorption in kesterite solar cells.

2. Analytical modeling methodology

Basically, the cornerstone of the proposed *CZTS* solar cell resides on engineering the absorber layer by using a graded band-gap profile. In this perspective, the *Se* content is increased with the *CZTS* layer thickness increase to reach its maximum in the *CZTS/Mo* interface as it is shown in Fig. 1 (a). This figure depicts the cross-sectional view of the proposed structure with an amended *CZTS* layer, where $E_g(y)$ represents the gradual band-gap in the *y* direction. Besides, the graded band-gap shape is suggested with a linear profile, as it is shown in Fig. 1(*b*).

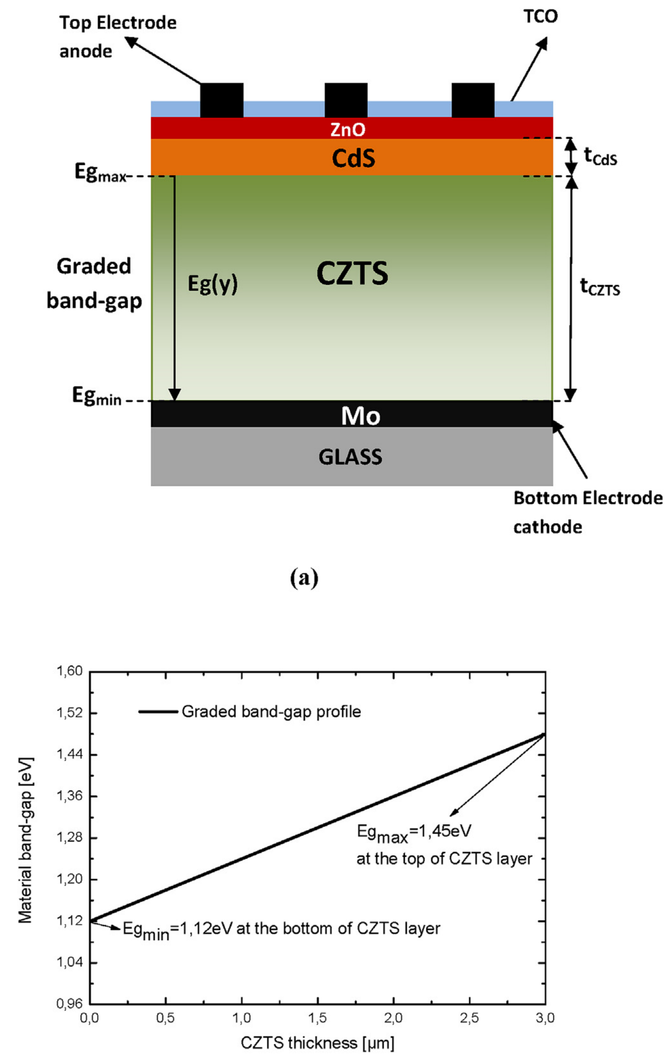
It is to note that numerous experimental studies have proved the possibility to adjust the *CZTS* material band-gap in the range of *1.5eV* and *1eV* by increasing the *Se* composite from $x = 0$ to $x = 1$ [16–18].

The investigated design is considered with *P-N* heterojunction chalcogenide thin-film design where the *CdS* layer acts as buffer layer in the top of the analyzed design. Moreover, glass coated *Mo* is used in the solar cell bottom, where the rear contact can be realized by the *Mo* metal, whereas at the top of the solar cell the front finger contacts can be formed on the *AZO* film which behaves like a good *TCO*.

For our analytical modeling, the parameter t_{CZTS} represents the *P-CZTS* absorber region thickness, t_{CdS} is the *n-CdS* layer thickness and $E_g(y)$ refers to the material band-gap variation as function of the thickness where Eg_{min} and Eg_{max} are the *CZTS* material band-gap values in the top and bottom of the amended absorber layer, respectively.

2.1. Analytical model of the photocurrent

The analytical current-voltage formulation of the investigated *CZTS*-based solar cell under illumination can be given by the following expressions [19].



(b)

Fig. 1. (a) Cross-sectional view of the proposed *CZTS*-based solar cell with graded band-gap aspect, (b) graded band-gap profile in the *CZTS* absorber layer.

$$I(V) = I_{ph} - I_s\left[e^{\frac{V-IR_s}{nV_{th}}} - 1\right] - \frac{V - IR_s}{R_{sh}} \tag{1}$$

where, *q* is the electron charge, V_{th} represents the thermal voltage, R_s and R_{sh} are the series and shunt resistances, respectively, *n* is the ideality factor, I_s refers to the saturation current and I_{ph} represents the photocurrent which is wavelength dependent.

In order to estimate the photocurrent, we need to calculate the *CZTS* solar cell optical parameters. In this perspective, we exploit a well-known expression of the absorption coefficient as a function of wavelength for un-polarized light provided by Tauc et al. model [20], which is considered as a good approximation that reproduces the experimental results associated with chalcogenide materials for direct band–gap transitions. In this context, the materials absorption coefficient can be estimated from the following expression [20–25].