# Contribution to the study of a CdS / CZTS-based solar cell with a gradual BSF layer

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Thin-film solar cells are currently the subject of several research works aimed at achieving the best relationship between energy and cost efficiency. The objective of this work is to improve the performance of a thin film solar cell based on CdS / CZTS by introducing a gradual layer on the back surface (Back Surface Field) in order to reduce the recombination losses in the back face and therefore increase the efficiency of photovoltaic conversion. The results obtained show that the addition of a back surface field (BSF) has a remarkable influence on the characteristics and the electrical performance of the solar cell. This results into an improvement in the values of the short-circuit current and of the open-circuit voltage, as well as the conversion efficiency with acceptable quantities. This study shows that, for an absorbent layer thickness of 2.42 µm, the BSF layer improves the photovoltaic conversion efficiency from 16.93% (cell without BSF) to 18.5% (for a cell with BSF).

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*Keywords:* Solar cell, CZTS, Absorbent layer, Gradual BSF, Performance

## 1. Introduction

Thin-film solar cells that use Cu2ZnSnS4 represent the most promising approach to reduce their production costs. Apart from some minor drawbacks, especially low efficiency, CZTS has several advantages such as easy processing on the one hand, excellent stability and high radiation resistance on the other hand [1, 2]. This cell is currently characterized by an average efficiency of 15% and a very high lifetime.

Cadmium sulfide (CdS) is widely used as a buffer layer for CZTS-based thin film solar cells. The optical gap of CdS is 2.42 eV offers a large window of absorption of solar radiation on the absorption layer in CZTS. More recently, research on CZTS solar cells without CdS has increased in order to decrease production, recycling costs and to diminish cadmium toxicity (Cd) [4]. Concerning these factors, there is compatibility between the CZTS absorption layer and other wide band-gap buffer layers. Zinc sulfide (ZnS) prepared by chemical bath deposition (CBD) turns out to be an attractive alternative to CdS in combination with CIGS absorbers [1, 2]. This is due to their wide band gap of the order of 3.68 eV and non-toxicity to the environment.

Several research studies have been launched in order to improve electrical characteristics (particularly efficiency); this framework was oriented towards improving the conventional CZTS (Se) structure and proposing new structures. Some of this work is based on the combination of CZTS with layers of other materials; CZTS / Si (C. Malerba et al 2019) [1] and (K.Kim et al 2017) [2], CBTS and CZBS (A.Ghobadi et al 2020) [3] and (Sadanand et al 2021) [4]. Other works focus on adding a layer of the abrupt BSF back surface field (Md S Rana et al 2021) [5], A Cherouana 2018 [6].

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The purpose of adding an additional layer or creating a rear or front surface field is to reduce the recombination rate and therefore increase the photocurrent and photovoltaic conversion efficiency.

Based on this recent research, the work presented in this manuscript revolves around adding a gradual layer to the BSF back surface.

The numerical simulation study is presented the performance of the CdS / CZTS (Se)-based gradual BSF layer solar cell. This research work is centered on the study of the gradual effect of BSF layer on the electrical parameters of CdS / CZTS (Se)-based solar cells.

The results clearly indicate that the gradual BSF layer improves the different performances of the cell under study.

## 2. Presentation of the BSF gradual layer solar cell:

The choice of materials for achieving a gradual structure is guided by the optical and electrical properties of the two materials, in particular by the values of their forbidden band.

The cell structure under study is shown schematically in FIG. 1. Comparing with the conventional structure of the cell based on CZTS, this structure shows the presence of an additional layer; the gradual BSF layer in CZTS (Se).

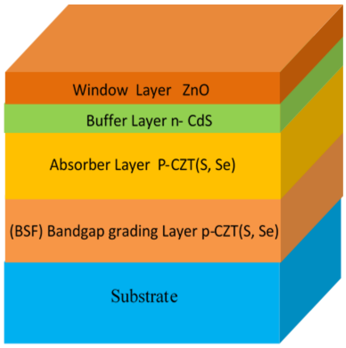


*Fig. 1. Structure of the CdS/CZTS/ CZTS(Se) graded BSF solar cell.*

The previous structure is made up of five main layers (from bottom to top);

- Substrate.
- Gradual BSF layer: with p-type conduction in CZTS (Se) with a variable gap of 1 to 1.5 eV.
- Absorbent layer: with p-type conduction in CZTS.
- Buffer layer: with n-type conduction in CdS.
- Window layer: a layer of transparent ZnO conductive oxide.

## 3. Calculation of the photocurrent

In this section, we will give the basic elements of our model. These are the current equations obtained by solving the one-dimensional continuity equations [8,9,10,11].

To determine the current density in the cell, one has to solve the continuity equation in the two regions i.e. the p region (CZTSe) and the n region (CdS).

These two currents will add to the current of the space charge zone.

$$J_{ph}(\lambda) = J_p(\lambda) + J_n(\lambda) + J_{dr}(\lambda) \tag{1}$$

### 3.1. Photocurrent density in region n (CdS)

In the case considered, the buffer layer is an n-type zone, the photocurrent is essentially a minority hole current, the electric field is zero and the continuity equation becomes [8]:

$$\mathrm{D_p}\frac{d^2\Delta p}{dx^2} - \frac{\Delta p}{\tau_p} + g_1(x,\lambda) = 0 \tag{2}$$

With;
$\Delta P$**:** Concentration of excited minority carriers
$D_P$**:** Hole diffusion coefficient
$\tau_P$**:** Hole carrier lifetime
$g_1$ (x, λ): Optical generation rate in layer n (CdS).
After calculating, the photocurrent in region n will be expressed by:

$$J_p(\lambda) = D_p \frac{d\Delta p}{dx}\bigg|_{x=d_1} \tag{3}$$

### 3.2. Photocurrent density in the p region (CZTS)

The continuity equation in the p-CZTS region is expressed by:

$$\mathrm{D_n}\frac{d^2\Delta n_1}{dx^2} - \frac{\Delta n_1}{\tau_n} + g_2(x,\lambda) = 0 \tag{4}$$

$\Delta n_1$: Concentration of excess electrons in the p-CZTS region.
$D_n$: Electron diffusion constant.
$\tau_p$: Electrons carrier lifetime.
$g_2$ (x, λ): Optical generation rate in the p layer (CZTS).
The general solution of equation (4) is given by:

$$\Delta n_1 = C_1 \exp\left(\frac{x}{L_n}\right) + C_2 \exp\left(-\frac{x}{L_n}\right) + \frac{Q_0}{D_n}\exp(-\alpha(\lambda)x) \tag{5}$$

With: $Q_0 = -\frac{\alpha(\lambda)}{\alpha(\lambda)^2 - L_n^2}$

$$J_n = D_n \frac{d\Delta n}{dx}\bigg|_{x=d_1+w} \tag{6}$$

The calculation of the current density in the region p (CZTS) ($J_n$) requires the determination of the constants $C_1$ and $C_2$ of equation 5 that will be calculated in detail in the following part.

### 3.3. Gradual region (BSF) p-CZTS (Se)

The continuity equation in the band gap gradient region:

$$\mathrm{D_n}\frac{d^2\Delta n_2}{dx^2} + \mu_n\xi\frac{\mathrm{d}\Delta n_2}{dx} - \frac{\Delta n_2}{\tau_n} + g_3(x,\lambda) = 0 \tag{7}$$

The driving electric field created by the band gap gradient is expressed as follows:

$$\xi = \frac{\mathrm{Eg_3 - Eg_2}}{\mathrm{d_3}} \tag{8}$$

With:
$\Delta n_2$: Concentration of excess electrons in the gradual band gap region.
$g_3$ (x, λ): Generation rate of carriers in the p layer (CZTS (Se)).
$g_3$ (x, λ) is given by [7,9]:

$$dc = (h\nu - Eg_2) / \xi \tag{9}$$

The rate of carrier generations in the gradual layer p (CZTS (Se)) depends on the value of the thickness of the gradual layer, it can be determined by;

a) for $x \leq d_c$

$$g_3(x,\lambda) = \alpha_0(h\nu - Eg_2 - \xi x)^{\frac{1}{2}} I_3 exp\left\{\alpha_0 \frac{2}{3\xi}[(h\nu - Eg_2 - \xi x)^{\frac{3}{2}} - (h\nu - Eg_2)^{\frac{3}{2}}]\right\} \tag{10}$$

with $I_3 = I_2 \exp(-\alpha d_2)$

b) for $x > d_c$

$$g_3(x,\lambda) = 0 \tag{11}$$

Equation (7) result is:

$$\Delta n_2 = C_3 exp(X_1 x) + C_4 \exp(X_2 x) + \frac{1}{X_1 - X_2}(\mathrm{Q}_1(\mathrm{x}) \exp(X_1 x) + \mathrm{Q}_1(\mathrm{x}) \exp(X_2 x)) \tag{12}$$

$$X_1, X_2 = \frac{q}{2kT}\xi \pm \left[(\frac{q}{2kT}\xi)^2 + \frac{1}{L_n^2}\right]^{1/2} \tag{13}$$

with

$$Q_1(x) = -\frac{1}{D_n}\int_0^x \exp(-X_1 x) g_3(x,\lambda) dx \tag{14}$$

$$Q_2(x) = \frac{1}{D_n}\int_0^x \exp(-X_2 x) g_3(x,\lambda) dx \tag{15}$$

The constants are determined from the following boundary conditions [8]:

$$\begin{cases} \Delta n_2 = 0 & x = d_1 \\ D_n \frac{d\Delta n_1}{dx} = D_n \frac{d\Delta n_2}{dx} + \mu_n \xi \Delta n_2 & x = d_2 \\ \Delta n_1 = \Delta n_2 \exp\left(-\frac{\Delta E_C}{KT}\right) & x = d_2 \\ D_n \frac{d\Delta n_2}{dx} + \mu_n \xi \Delta n_2 = S_n \, \Delta n_2 & d_3 = 0 \end{cases} \tag{16}$$

The current in the p region will be determined by:

**3.4. Current in the space charge zone**

The density of the photocurrent in the charge zone depends on the number of photons absorbed:

$$J_{dr}(\lambda) = qI_0 \exp(-\alpha(\lambda) d_1)(1 - \exp(-\alpha(\lambda) w) \tag{17}$$

**3.5. Parameters**

Physical parameters of different layers of the proposed CZTS solar cell:

*Table 3.1. Parameters of the CdS / CZTS standard cell [4, 5, 10,11].*

| **Parameter** | **CZTS(Se)** | **CdS** |
|---|---|---|
| Thickness, W (nm) | 2500 | 80 |
| Band gap, Eg (eV) | 1.45 | 2.4 |
| Electron affinity, $\chi$(eV) | 4.5 | 4.2 |
| Dielectric permittivity, $\varepsilon_r$ | 10 | 9 |
| Effective Density of states, $N_C$($cm^{-3}$) | $2.2\times 10^{18}$ | $2.2\times 10^{19}$ |
| Effective Density of states, $N_V$($cm^{-3}$) | $1.8\times 10^{19}$ | $1.8\times 10^{18}$ |
| Electron mobility, $\mu$e ($cm^2$/Vs) | 100 | 100 |
| Hole mobility, $\mu$p ($cm^2$/Vs) | 25 | 25 |
| Donor Concentration, n ($cm^3$) | 0 | $3.0\times 10^{16}$ |
| Acceptor Concentration, p ($cm^3$) | $1.0\times 10^{17}$ | 10 |
| Surface recombination velocity of electrons (cm/s) | $10^7$ | $10^7$ |
| Surface recombination velocity of holes (cm/s) | $10^7$ | $10^7$ |
| Capture Cross section area of electrons ($cm^2$) $\delta_e$ | $4.4\times 10^{-16}$ | $4\times 10^{-18}$ |
| Capture Cross section area of holes ($cm^2$) $\delta_h$ | $4.4\times 10^{-15}$ | $4\times 10^{-18}$ |
| Defect density, Nt (cm-3) | $10^{16}$ | $10^{18}$ |

## 5. Results

### 5.1. Effect of surface recombination on the spectral response of standard CdS / CZTS-based solar cell

To justify the choice of adding a BSF layer, we will first present the simulation results of a standard CZTS-based solar cell in order to show the degradation of the standard performance cell due to recombination.

To study the internal performance of the cell, it is recommended to study the variation of the spectral response as a function of the wavelengths of the absorbed photons. The spectral response makes it possible to evaluate the collection efficiency of a solar cell as a function of the incident light wavelength.

Figure 2 represents the variation of the spectral response of the standard CdS / CZTS solar cell for different values of surface recombination.

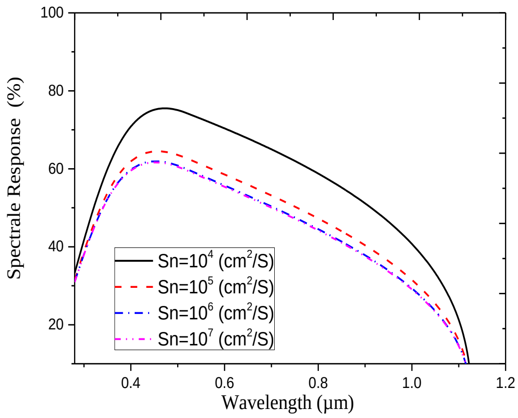


*Fig. 2. Spectral response of standard CdS / CZTS-based solar cell for different values of surface recombination.*

Figure 2 shows that, under the effect of surface recombination, the spectral response has a noticeable variation throughout the absorption spectrum. Therefore, to improve the performance of this type of cell (CZTS), several studies have been carried out in order to reach competitive yields with those of CIGS. In this study, our proposal is oriented towards the insertion of a gradual band gap BSF layer.

### 5.2. Graduated BSF solar cell based on CdS / CZT (S, Se)

In FIG. 3, and in order to demonstrate the effect of surface recombination on the nature of the absorbent layer, the variation in the spectral response of the standard CZTS solar cell and with gradual BSF layer (gradual bandgap) is plotted**.**

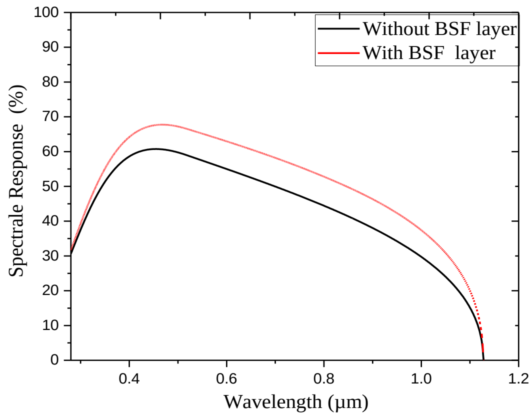


*Fig. 3. Spectral response of standard CdS / CZTS solar cell and CdS / CZTS / CZT gradual BSF layer cell (S, Se).*

Analysis of Fig. 3 shows that, for the CdS / CZTS / CZT (S, Se) BSF gradual layer solar cell; the spectral response displays a significant improvement in the range of wavelengths from 0 µm to 1.1 µm. The photo carriers that reach the gradual layer will be accelerated by the electric field of this area, which leads to an increase in the number of these carriers and hence there is a rise in cell current, which is mainly due to the BSF layer which reduced the rate of loss by surface recombination.

### 5.3. Effect of surface recombination on the electrical characteristics of the BSF-coated CZTS cell

To analyse the effect of surface recombination on the CZTS-based solar cell, and show the influence of this parameter on the performance of the two cells examined (standard cell and cell with BSF), we have plotted in Figures 4, 5, 6 and 7 the variation of the electrical parameters (current, open circuit voltage, form factor and conversion efficiency) as a function of the surface recombination for the standard solar cell based on CZTS and with a gradual BSF layer**.**

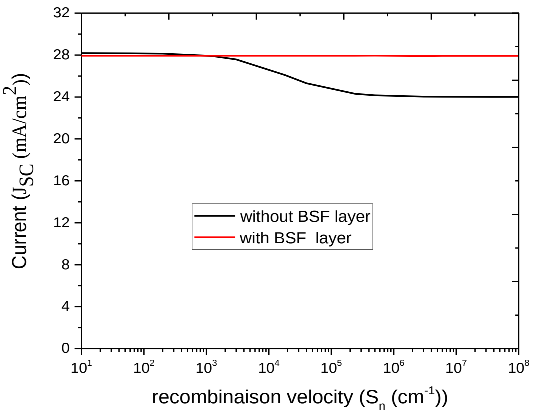


*Fig. 4. Effect of surface recombination on the graded BSF layer CZTS cell photocurrent.*

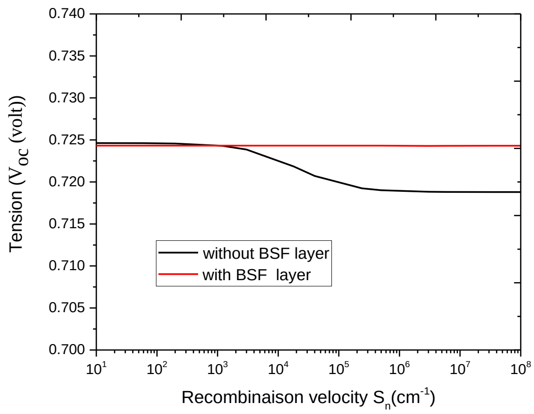


*Fig. 5. Effect of surface recombination on the open circuit voltage of the gradual BSF layer CZTS cell.*

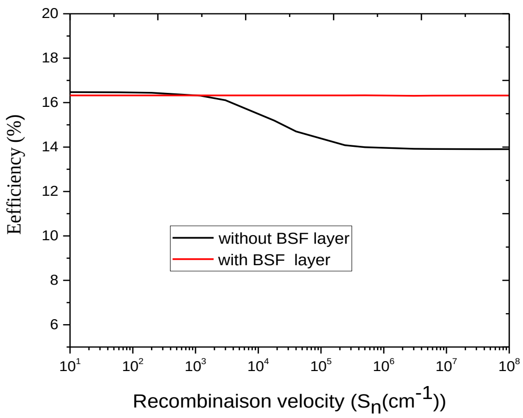


*Fig. 6. Effect of surface recombination on the form factor of the graded BSF layer CZTS cell.*

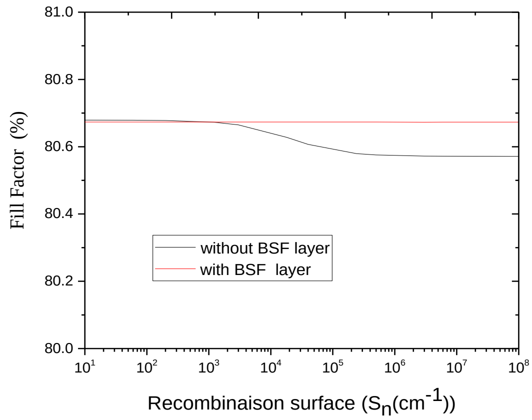


*Fig. 7. Effect of surface recombination on the photovoltaic conversion efficiency of the gradual BSF layer CZTS cell.*

The analysis of Figures 4 - 7 shows a decrease in the photocurrent compared to the variation in the value of surface recombination. This decrease is more remarkable and quicker in the case of the standard cell. The reason for this difference for a graded BSF layer cell is the electric field which lowered the value of the recombination. For the curve that corresponds to the standard cell, the effect of the superficial realliance of the absorber on the photocurrent value is important when the values of the remerging rate are beyond$10^4\ cm^{-1}$.

Hence, it can be said that adding a BSF layer has a very important role in improving the current.

We have shown that the recombination current can be decreased by the back electric field. This field influences the separation of carriers, which is necessary for cell function.

The effect of surface recombination on the voltage is less weak compared to the photocurrent. For the gradual cell, the effect of the realliance is almost non-existent; this is justified by the fact that the remerging is linked to the photocurrent, so the voltage is only slightly affected.

The surface recombination has a remarkable effect on the photovoltaic conversion efficiency, and this is due to the direct relationship between photocurrent and efficiency.

**5.4. The electrical characteristics:**

Table 2 illustrates the electrical characteristics of the two cells examined (standard and BSF graded layer).

*Table 2. Characteristics of a BSF gradual layer solar cell.*

| **Performance** | Short circuit current ($J_{cc}$ (mA / cm$^2$)) | Open circuit voltage ($V_{co}$ (V)) | Efficiency $\eta$ (%) | Form factor (FF (%)) |
|---|---|---|---|---|
| **Standard cell** | 24 | 0.718 | 13.9 | 80.5 |
| **Gradual BSF layer cell** | 28 | 0.724 | 16.32 | 80.7 |

The analysis of the results presented in the preceding table shows that; the density of the short circuit current increases from 24 mA / cm$^2$ for a standard cell based on CZTS to 28 mA / cm$^2$ for a cell with a gradual BSF layer, which shows an improvement in the photovoltaic conversion efficiency from 13.9% to 16.32%. The open circuit voltage and the form factor undergo a slight increase.

## 6. Conclusion

In this paper, we have studied the interest of adding a BSF layer (back surface field) stepwise in a CZTS-based thin-film solar cell in order to minimize the effect of losses by surface recombination and improve the performance of the photovoltaic cell.

The deposition of a gradual BSF layer shows a significant development on the various electrical parameters of the CdS / p-CZTS / p-CZTS (Se) based solar cell.

The addition of a back surface field on the solar cell has a noticeable influence on its electrical characteristics and performance. There is an enhancement in the short circuit current and open circuit voltage values as well as the conversion efficiency with acceptable magnitudes.

For example, the photocurrent shows an augmentation of 24-28 mA / cm2. Moreover, the photovoltaic conversion efficiency increases from 13.9% for a standard solar cell to 16.32% for one with a gradual BSF layer.

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