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Interface defects within the junction region and its effect on the electrical and optical properties of a heterojunction solar cell

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ABSTRACT

The simulation model used in this study is the heterojunction solar cell with SnS absorption layer using the AFORS-HET simulation program. Where the effect of interface defect density (Nit) and the location of these levels within the interface on the electrical and optical properties was studied. Through the study, we learned the effect of the locations of the energy levels for defects within the junction, and it was found that the largest effect of the defects is within the locations of the deep energy levels, D.deep traps and A.deep traps within the junction. After that, the effect of interface defect density and its relationship to thickness and impurities concentration of both the buffer and absorption layer were studied, as the increase in the thickness of the absorption layer indicated a clear decrease in the effect of the density of the interface cases, otherwise the increase in the thickness of the buffer layer did not reduce the effect of these defects. The effect of the interface defect density increases with increasing the concentration of impurities in the SnS absorption layer, the effect of the density of the interlayer defects decreases with the increase in the concentration of impurities in the buffer layer.

1. Introduction

Solar energy is a clean and efficient renewable energy source, and harvesting it through the photoelectric effect (converting light energy into electrical energy) has the potential to combat global warming, which is a major cause of worry throughout the world. Photovoltaics were first investigated six decades ago in order to harness solar energy. During this investigation, numerous materials such as Si, CIGSSe, CdTe, CZTSSe, Perovskites, and other materials appeared as absorbent layers in solar cells, and Si solar cells now dominate the PV industry [1] . CIGSSe and CdTe-based solar cells have demonstrated higher efficiency in thin film solar cells [2] ,[3] but indium (In) is rare in CIGSS, and the toxicity of cadmium (Cd) in CdTe has prevented their widespread usage. CZTSSe-based chalcogenide, on the other hand, was utilized as a substitute for CIGSSe-based solar cells. CZTSSe absorption layer solar cells have a maximum efficiency of 12.4 % [4]. However, the primary challenge with this form of solar cell is achieving optimum conversion efficiency by controlling the composition of this compound during manufacturing Other materials utilized as an absorption layer in solar cells using thin film technologies that have been extensively investigated and studied include SnS, [3],FeS2, Cu2O[5]and Cu2S [6], although their conversion efficiencies are still significantly lower than expected [7].

The ability to absorb light as much as possible in order to excite electrons to higher energy states and the ability to transfer those excited electrons from the solar cell to the external circuit are the two most important points to consider when choosing a material for an absorbent layer in solar cells [8]. Chalcogenide compounds, which are made up of elements from the periodic table's fourth and sixth groups IV and VI, are well-known semiconductors that have attracted the interest of many researchers due to their narrowing energy gap and ability to be employed in PV devices and solar cells [9]–[11]. Because of its unique features, such as non-toxicity and abundance in nature, an optimal energy gap of 1.3 eV, and a high absorption coefficient more than $10^4 cm^{-1}$, SnS tin sulphide has been identified as a viable option as an absorption layer in thin-film solar cells. SnS is a good material for thin-film solar cells because it has a good energy gap and a high absorption coefficient [12][13]. The electrical and optical properties of SnS-based solar cells have been experimentally studied by achieving a conversion efficiency of 4.36% solar cells [14]. In order to achieve higher solar cell efficiency, it is necessary to understand the device's mechanism and behavior. As a result, in addition to experimental studies, a theoretical study of solar cells is necessary to determine the optimal parameters for the experimental study in order to achieve maximum solar cell efficiency. The recombination losses of the photovoltaic charge carriers have a direct impact on the efficiency of solar cells, according to theoretical research. As a result, in order to enhance the efficiency of solar cells, charge carrier recombination must be controlled [15].

The effect of interface state density between SnS / CdS in a heterojunctoin solar cell and its relationship with other parameters such as thickness and carrier concentration in each layer were simulated in this paper using the AFORS-HET-1D software designed to simulate heterojunctoin device characteristics.

2. Cell simulation and structure:

The simulation in this work is based on the AFORS-HET-D program, which is a simulation program in numerical analysis that is widely used to study heterojunctoin solar cells, It is one of the programs capable of numerically solving Poisson's equation and continuity of holes and electrons. Whereas, the AFORS-HET program was used to study the effect of interface defect density between SnS / Cds, which is the only effect in simulation in order to understand the effect of these defects on the electrical and optical properties, And correlate their effect with other parameters of the cell, such as thickness and concentration of impurities for both the Cds buffer and SnS absorption layer. The transport across the interface is modeled by thermal emission, based on perfect simulations, bulk defect was not inserted into the window and absorption layer in order to make the simulation as simple as possible, the effect of shunt resistance and series resistance was not taken into account, In all cases of simulation. Both front contact and back contact are designated as "flat band", which is purely ohmic connection.

The simulations were performed by specifying the solar cell composition and the electrical and optical parameters of each layer as input media for the simulation. In this study, we consider the installation of SnS thin-film solar cells whose layers consist of the following materials: The window layer n-ZnO, n-Cds buffer and p-SnS absorber are shown in Fig.1a. The schematic structure of the cell is shown in Fig. 1. b. The basic input parameters used in the simulation are adopted, as shown in Table 1. The illumination is set to the global AM1.5 standard and the operating point is set to 300K.

Table 1 shows the basic parameters involved in simulation solar cell

Parameters	n-ZnO [15] ,[19]	n-CdS [15], [20], [19]	p-SnS [15]–[17]
Thickness, W (nm)	200	80	2000
Relative permittivity	9	10	13
Electron affinity (eV)	4.5	4.4	4
Eg (eV)	3.35	2.42	1.3
Nc (cm-3)	2.2E18	2.2E18	1.18E18
Nv (cm-3)	1.8E19	1.9E19	4.76E18
Electron mobility($cm^{-2}.V^{-1}.s^{-1}$)	100	160	15
Hole mobility ($cm^{-2}.V^{-1}.s^{-1}$)	25	15	100
Donor concentration (cm-3)	1E18	1E17	0
Acceptor concentration (cm-3)	0	0	1E16
defect (cm^{-3}) bulk	0	1E17	0
)interface defect(G.D.) (cm^{-2}		1E14	

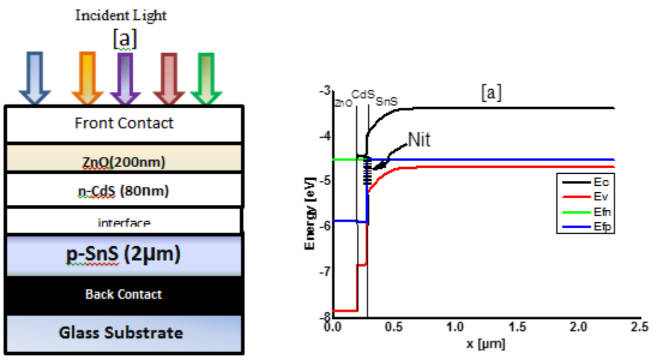

Fig. 1: shows (a) the solar cell structure and (b) the band diagram at equilibrium

3. Results and discussion

1- The location of the density of the interface defects in the region of depletion:

The density of the interface defects and the location of the defect level has a clear effect on the performance of the solar cell, as the density of the interface states was changed from 1E10 to 1E14cm-2 at each location, and the types of defects were accepted-like and donor-like within the interface, and each of them was divided into shallow traps and deep traps, this depends on their location in the junction, the results showed a decrease in Voc, Jsc, FF and Eff with an increase in the density of interface defects as shown in Figure 2, and this decrease in performance is due to the increase in the surface recombination rate at the junction. As for the effect of the location and type of the defects' energy levels, it was clear, as it was noted from the results that shallow traps D. was more effective on Voc than other defects in different locations with the stability of Jsc and FF when D.shallow traps and A.shallow traps, However, the decrease in Jsc and FF was evident in D. deep traps and A. deep traps, and this was evident in its effect on the conversion efficiency. This is in agreement with the study of researcher A. S. Chouhan, S. Srivastava and others[21,22].

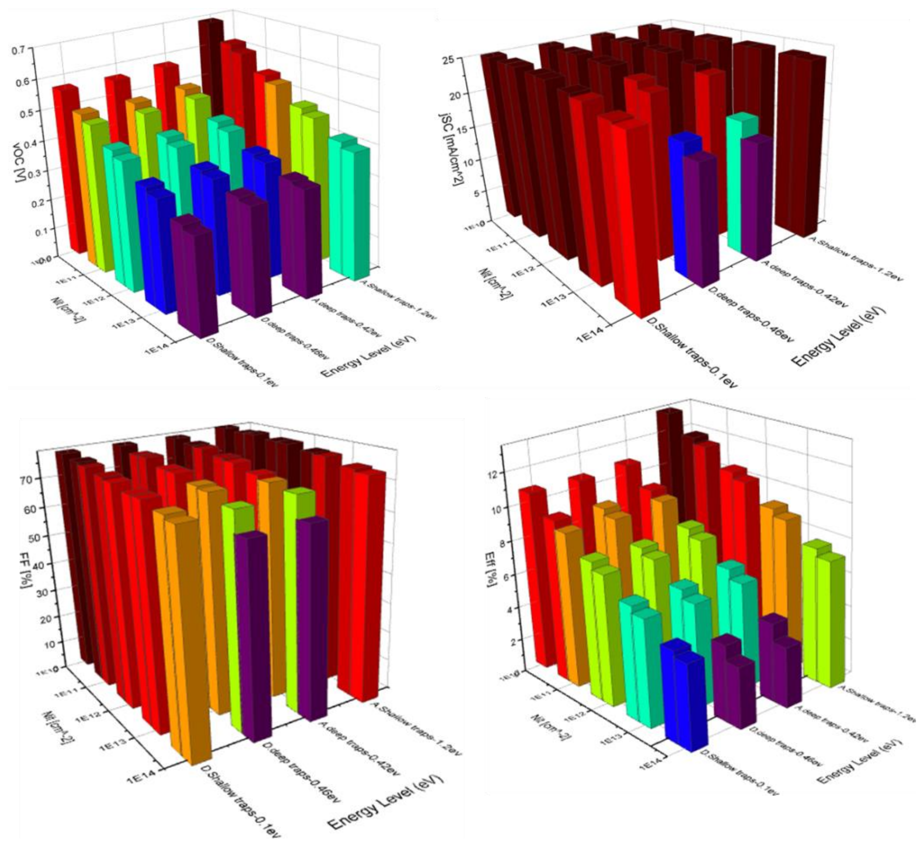

Fig. 2: shows the effect of the location of the energy states and the density of the interface states on the performance of the solar cell, all location above C.B, from 0.1ev to 1.2ev

Also, we showed a decrease in Jsc with an increase in the density of the interface states, due to the increase in surface recombination, which led to a decrease in the concentration of photo-generated carriers, thus, the quantum efficiency decreases at wavelengths less than 500nm, as for the apparent decrease in the quantum efficiency at the interface density between 1E13 and 1E14 cm^{-2} within the wavelengths confined between 500nm-800nm, This is due to the decrease in The diffusion length of carrier within this range and this was evident in Figure3.a As for the decrease in Jsc, it was clear as the defects level approached the depth of the gap, due to the increase in the chances of recombining the photo-generated carriers as they approached the depth of the gap. This is evident by increasing the quantitative efficiency as the defect level locations approach V.B and C.B as shown in Fig.b3.

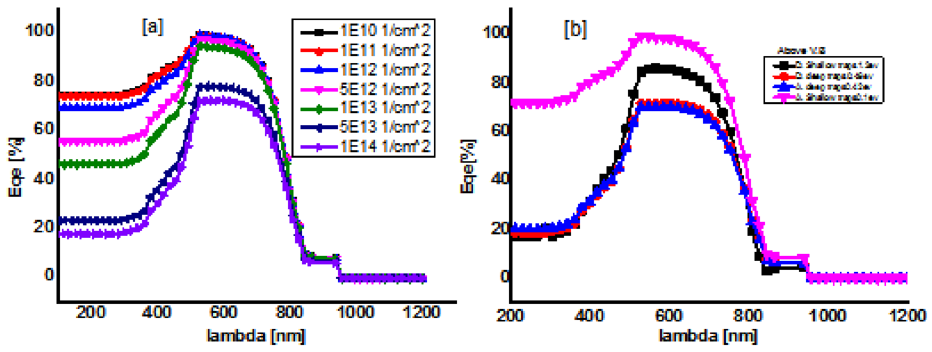

Fig. 3: shows the change of quantum characteristics with change [a] The density of the states of interface defects and [b] the location of the energy level of the defects.

As for the decrease in Voc and FF, with an increase in the density of interface defects, shown in the previous figure 2, This was attributed to the increased surface recombination between SnS/Cds and thus the decrease in the concentration of the holes and electrons on sides junction. This was evident in Fig. 4. a. b , .

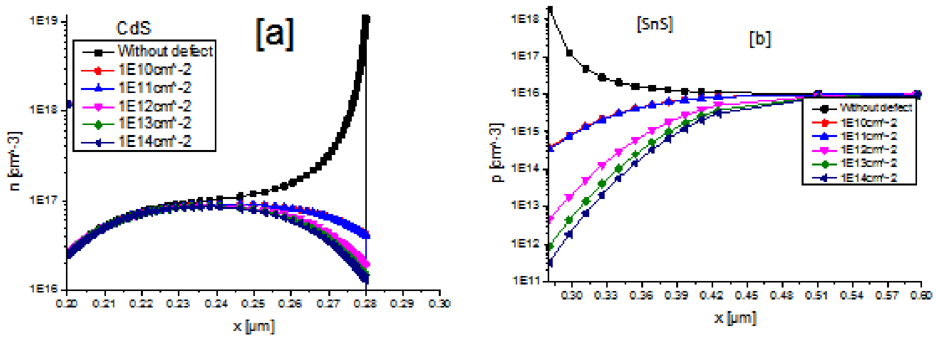

Fig. 4: shows the change in the concentration of charge carriers [a] electrons and [b] holes with the change in the density of the interface states

2. The density of the interface states changes with the thickness of the absorber layer:

Figure 5 illustrates the effect of changing the density of the interface states between SnS / Cds on the electrical and optical properties at each thickness of the absorber layer, the thickness was changed from 600 to 9000nm, and in contrast, the case density of the interface defects was changed from 1E10 to 1E14 cm^{-2}. The results showed that Voc and FF did not change with the change in thickness, but there was a change with the density of the interface states, where Voc decreased from 0.556 to 0.331 V and FF from 78.90 to 60.15%.As for Jsc, the change in it was evident with the change in thickness at the density of the defects less than $1E13cm^{-2}$, where the increase from 19.95 to $28.45mA/cm^{2}$, but this effect becomes very small when the density of the interface states is greater than $1E13cm^{-2}$ and the Jsc values decrease from 26.33 to 11.45 mA / cm^{-2} as the density of the interface states increases. Hence, the biggest influence on the conversion efficiency is the density of the interface states, as shown in Figure 5. This is in agreement with the study of researcher S. Ahmeda and others [23].

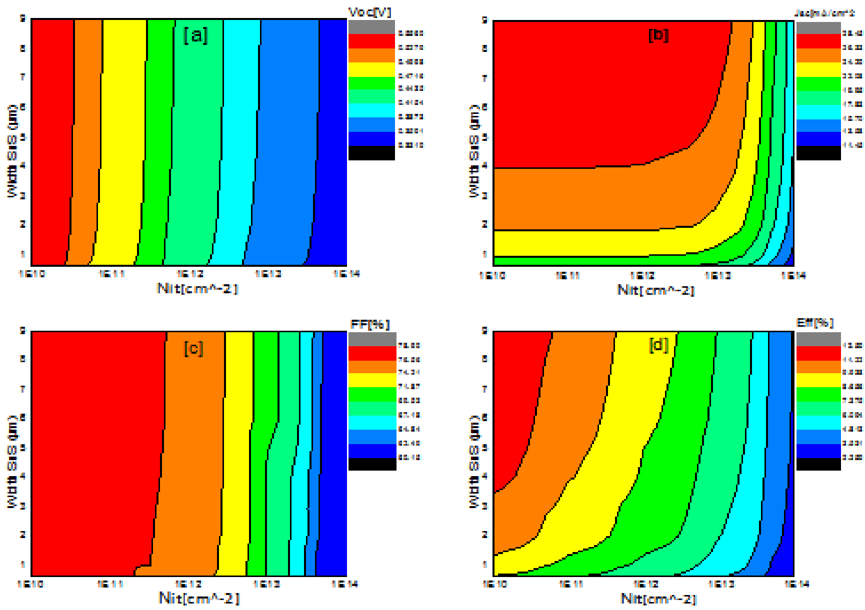

Fig. 5: shows the effect of the thickness of the absorption layer with the density of the interface states on the performance of the solar cell

The reason for the increase in Jsc at the density of defects of 1E10 cm^{-2} with the change in thickness is due to the large numbers of photons having wavelengths greater than 500nm being absorbed and contributing to the increase in the generation of electron-hole pairs and this was evident in Fig6.a Increasing quantum efficiency with increased thickness, Therefore, the increase in the conversion efficiency is apparent when the thickness of the absorber layer is greater than 2000nm. At the defect density of 1E14 cm-2, we observe that the Jsc is lower than at 1E10 cm-2, due to the increase in the recombination of the photogenerated electron-hole pairs and consequently the lower quantum efficiency at all wavelengths, as in Fig. 6b.

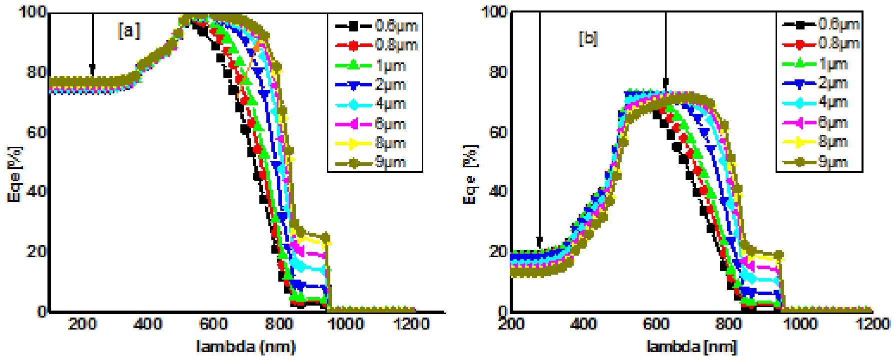

Fig. 6: shows the change of quantum efficiency at the density of the interface states[a] 1E10 cm^{-2} and [b] 1E14 cm^{-2} with the change in SnS thickness.

3. change density of the interface states with the thickness of the buffer layer CdS:

When the density of the interface states changes between SnS / Cds from 1E10 to 1E14cm^{-2} and the thickness of the buffer layer from 20 to 180 nm as shown in Figure 7, the results showed that Voc and FF did not change with the change of thickness, but there was a decrease from 0.55 to 0.323 V and from 77.75% to 60.06%, respectively, with an increase in the density of interface states, this is due to the decrease in the concentration of holes and electrons in the junction region between SnS/Cds as shown in the previous figure 4.a.b and the decrease in carriers is due to the surface recombination in interface region due to the increase in the density of the interface states Nit.

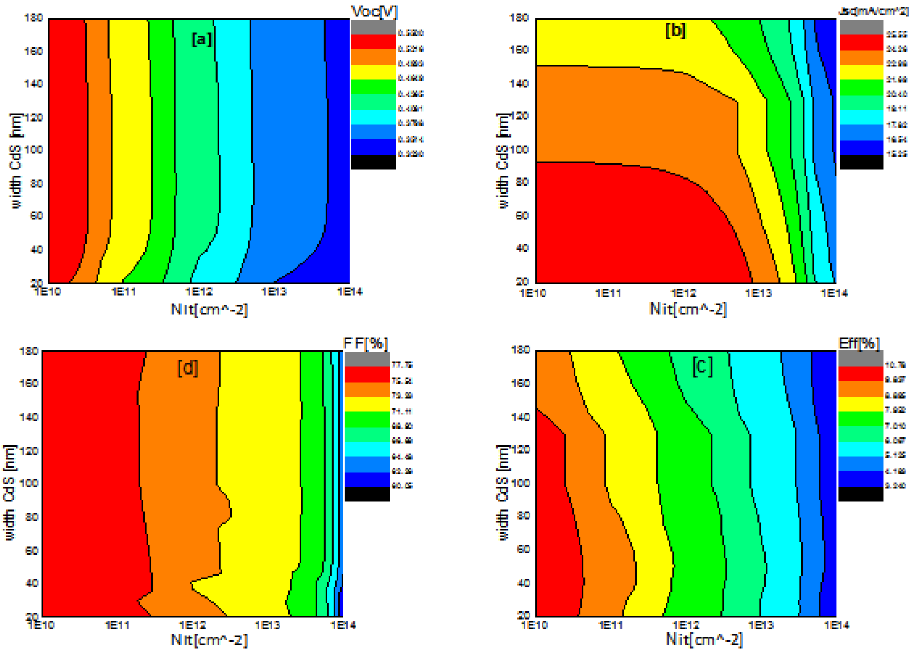

Fig. 7: illustrates the effect of buffer layer thickness and interface density on the performance of the solar cell.

The reason for the decrease of Jsc at the density of defects of 1E10cm^{-2} with the increase in the thickness of the buffer layer is due to the large numbers of photons having wavelengths less than 500 nm being absorbed before they reach the absorption layer, This contributes to a decrease in the generation of electron-hole pairs in the absorption layer and this was evident in Figure a. 8 in the region. (1). As for the defect density of 1E14cm^{-2}, we showed a decrease in the quantum efficiency with an increase in thickness in regions (1) and (2) of Figure 6.b, this is due to the increase in surface recombination and the decrease in the diffusion length of the charge carriers, and thus the decrease of Jsc.

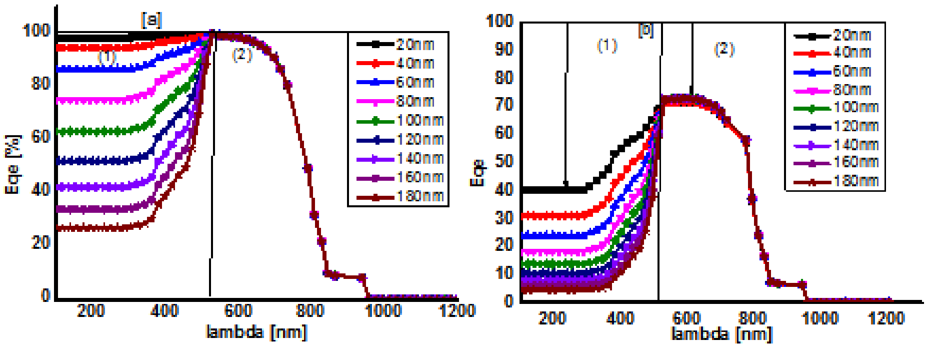

Figure (8) shows the change of quantum efficiency at the density of the interface states [a] 1E10cm^{-2}and [b] 1E14cm^{-2}with the change in the thickness of CdS.

4. Change density of the interface states with N_A:

By changing the density of the interface states with the concentration of impurities as shown in Fig. 9, it was found that both Voc and FF at the defect density of 1E10cm^{-2} obtained an increase with increasing the concentration of impurities from 0.514 to 0.5710 V and 71.85 to 78.70%, respectively. As for the density of interface defects of 1E14cm^{-2}, we notice a decrease in Voc from 0.4 to 0.343 V with an increase in the concentration of impurities. In general, the effect of the defect density increases with increasing the concentration of impurities, while the FF increases with increasing the density of the interface defects at 1E14cm^{-2} and with increasing the concentration of impurities.

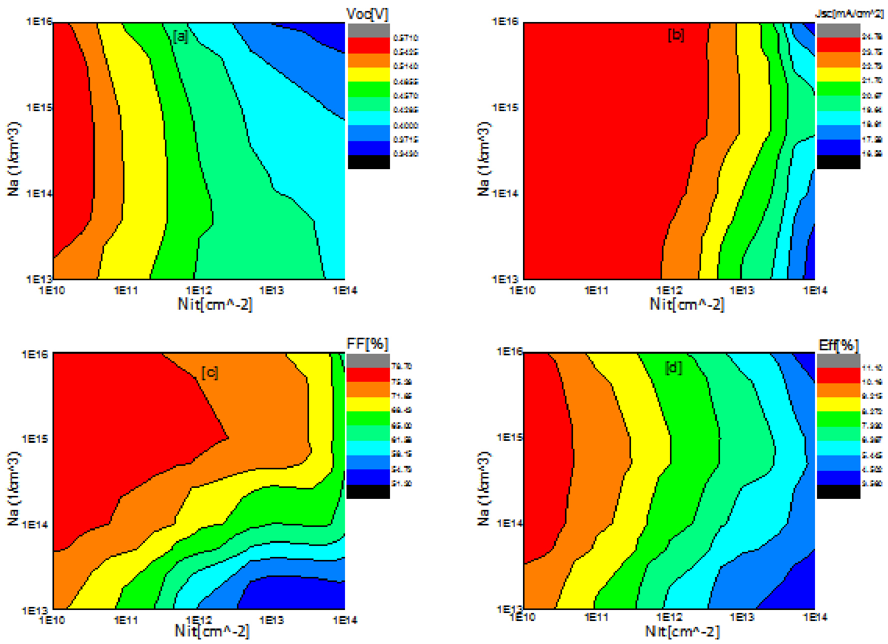

Fig. 9: shows the effect of the concentration of N_A impurities with the density of the interface states on the performance of the solar cell

When the concentration of N_A carriers in the absorption layer increases, this leads to a decrease in the reverse saturation current I_0 and thus leads to an increase in V_{oc}, However, the increase in the density of the interface states will be counterproductive due to the increase in the chances of recombining the carriers in the junction region and thus the decrease in the length of the carrier diffusion, which leads to an increase in the reverse saturation current and thus a decrease in V_{oc}, and these results are consistent with equation 1 and 2:

$$V_{oc} = \frac{KT}{q} \text{Ln} \left(\frac{I_L}{I_o} - 1\right) \approx \frac{KT}{q} \text{Ln} \left(\frac{I_L}{I_o}\right) \ldots\ldots.\ldots (2)$$

$$I_o = A \left[\frac{q\, D_e n_i^2}{L_e N_A} + \frac{q D_h n_i^2}{L_h N_D}\right] \ldots\ldots\ldots\ldots (1)$$

The decrease in Jsc at low interfacial density E10cm^{-2} is due to the decrease in quantum efficiency at wavelengths between 100 and 500 nm due to the recombination of photo-generated carriers within these wavelengths as shown in region (1) in Fig. 10.a. As for the short circuit current Jsc at the interface density of 1E14 1cm^{-2}, it increases with the increase in the concentration of Na carriers to 1E15cm^{-3} and after this concentration the value of Jsc begins to decrease and this is mainly due to the fact that the increase in the carrier density led to an increase in the generation of electron-hole pairs, these pairs decrease at the concentration of carriers greater than 1E15cm^{-3}, and this was evident through the quantum efficiency as shown in Figure 10.b, due to the low concentration of carriers and the decrease in the probability of collecting photo-generated electrons as shown in Figure 10.c.d.

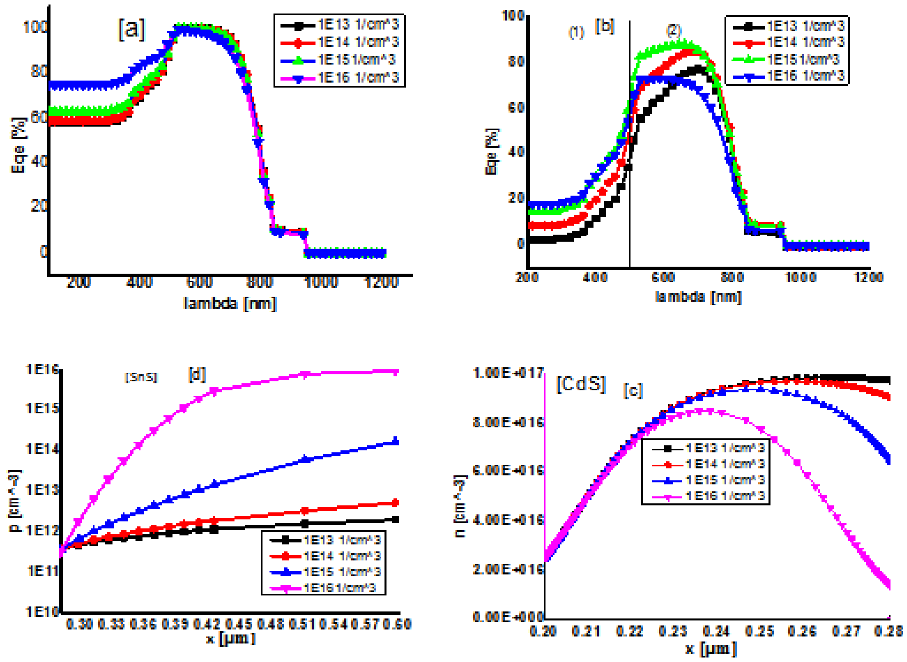

Fig. 10: illustrates [a] the process of recombining carriers within the region of depletion [b] the quantum efficiency at an interface defect density of 1E14cm^{-2} , [c] and [d] the concentration of the electrons and the holes with the concentration of the N_A carriers changes

5. change density of the interface states with N_D.

During the study of the effect of the interface states density between SnS/Cds with the change of the impurities concentration in the buffer layer, it was found in Fig. 11 that increasing the concentration of impurities leads to a decrease in the effect of the density of the interface defects on the electrical properties. Whereas, we observed that Jsc at the 1E10cm^{-2} interface defect density decreased from 25.10 to 23.84 mA/cm^2 with the impurity concentration increased. At the concentration of impurities less than 1E17cm^{-3} and the density of interface states 1E14cm, Jsc decreases from 18.82 to 15.05 mA/cm^2, After this concentration, Jsc begins to increase from 18.82 to 25.10 mA/cm^2. As for Voc and FF, they increase from 0.1480 to 0.682 V and from 67.63 to 82.40%, respectively, with the concentration of impurities increases and at low density of interface defects. And when the density of the interface defects greater than 1E13cm^{-2}, Voc and FF increase from 0.1480 to 0.6820 V and from 43.00 to 82.40%, respectively, with increasing the concentration of impurities, Consequently, all this led to a decrease in the conversion efficiency with an increase in the density of the interface defects, which increased with the increase in the impurity concentration.

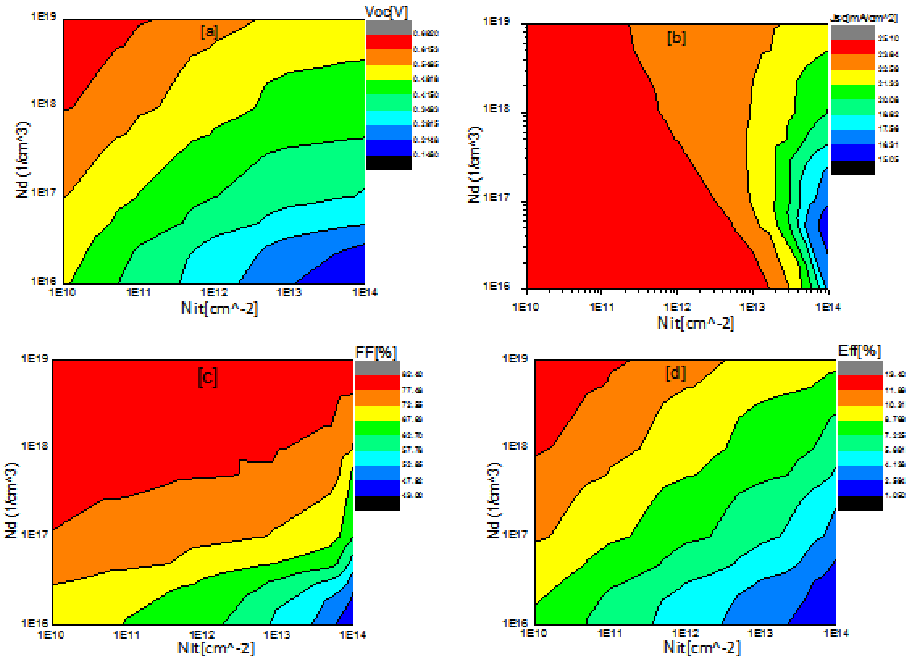

Fig. 11: shows the effect of the concentration of N_D impurities with the density of the interface states on the performance of the solar cell

The decrease in Jsc at the intensity of low interface defect states 1E10cm^{-2} is due to the decrease in quantum efficiency at wavelengths between 100 and 500 nm Due to recombination of photo-generating carriers within these wavelengths as is evident in region (1) in Fig. 12.a. Also, we observed a decrease in the effect of the of density states at 1E14cm^{-2} with an increase in the concentration of impurities greater than 1E17cm^{-3}, due to an apparent increase in the quantum efficiency within the lengths greater than 500nm, This is due to the increase in the diffusion length of the carriers with the increase in the concentration of impurities and this was evident in region (2) and (1) in Fig. 12. b, And it was also evident in Figure 12.c, which shows the increase of the electron charge carriers with the increase in the concentration of impurities in CdS, and thus the decrease in the concentration of the hole carriers in SnS as shown in Figure 12.d. As for Voc and FF, they increased with increasing the concentration of impurities at the density of the interface states 1E14 cm^{-2} due to the decrease in the amount of the reverse saturation current with the increase in the concentration of impurities.

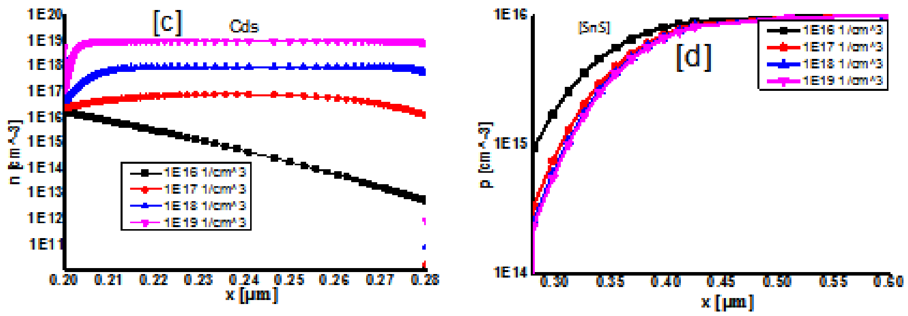

Fig. 12: illustrates the change of [a] the quantum efficiency at the density of interface defects of 1E10cm-2 and [b] the quantum efficiency at the density of interface defects of 1E14cm-2, [c] and [d] the concentration of electrons and holes with changing concentration Carriers N_D

Conclusions

When studying the effect of the density of interfacial defect states between SnS/CdS on the electrical and optical properties, As for the effect of the location and type of the defects' energy levels, it was clear and it was noticed from the results that D.shallow traps was more effective on Voc than other defects in different locations with the stability of Jsc and FF at D. shallow traps and A. shallow traps, however, the decrease in Jsc and FF was evident for D. deep traps and A. deep traps, and this was evident in its effect on the conversion efficiency. Also, we noticed the effect of changing the thickness of the buffer and the absorption very little when the density of the interlayer cases was greater than $1E13cm^{-2}$, and therefore the biggest influence on the conversion efficiency was the intensity of the states of interface defects. As for the change in the intensity of the cases of interface defects with the concentration of impurities N_A in the absorption layer, we observed the effect of the density of the interface defects decreased with increasing the concentration of the impurities to the concentration of $1E15cm^{-3}$, after this concentration, the effect of the density of the states of the interface defects increases, and this was evident through the electrical and quantum properties. As for the change in the density of the interface states and the concentration of impurities N_A in the buffer layer CdS, we observed a decrease in the effect of the interface states of defects with increasing the concentration of impurities.

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العيوب البينية ضمن منطقة المفرق وتأثيرها على الخصائص الكهربائية والبصرية لخلية شمسية ذات مفرق متباين

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الملخص

نموذج المحاكاة المستخدم في هذه الدراسة يتمثل بالخلية الشمسية المتباينة ذات اساس SnS باستخدام برنامج المحاكاة AFORS-HET , حيث تمت دراسة تأثير كثافة الحالات البينية N_{tr} وموضع هذه المستويات داخل السطح البيني على الخصائص الكهربائية و البصرية .وتعرفنا من خلال الدراسة على تأثير مواضع مستويات الطاقة للعيوب ضمن المفرق وتبين من ذلك ان اكبر تأثير للعيوب يكون ضمن مواضع الطاقة العميقة D.deep traps و A.deep traps داخل الفجوه. وبعد ذلك تم دراسة تأثير كثافة الحالات البينية وعلاقتها بسمك وتركيز الشوائب لكلا من طبقة المؤامة والامتصاص, حيث اظهرت الزيادة في سمك طبقة الامتصاص انخفاض واضح في تأثير كثافة الحالات البينية على خلاف من ذلك زيادة سمك الطبقة العازلة لم تقلل من تأثير هذه العيوب. اما حيز تأثير كثافة العيوب البينية يزداد مع زيادة تركيز الشوائب في طبقة الامتصاص SnS, وينخفض ذلك التأثير مع زياد تركيز الشوائب في الطبقة المؤامة.