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Effect of Defect Density in Solar Cell $Cu_2Te/CdTe/CdS:O/Zn_2SnO_4/FTO$ on Electrical Properties (I-V) Using SCAPS-1D Program

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***Abstract* - Defects in the Absorber Layer and other layers of the interlayer in Cadmium Telluride (CdTe) cells are detrimental to their efficiency and stability, the present work will focus on investigating the effect of these defects on their electrical properties (I-V), this work was chosen to simulate solar cells using SCAPS-ID program. The solar cell consisted of Cadmium Telluride (CdTe) as an Absorber layer with a thickness of 0.25µm and a Windows layer (CdS:O) with a thickness of 0.025µm and Buffer Layer (Zn_2SnO_4) with a thickness of 0.05µm a Transparent Conduction Oxide (FTO) Layer with a thickness of 0.1µm and a Back Reflection layer (Cu_2Te) with a thickness of 0.1µm. The best results obtained were: {V_{oc}=0.85V, J_{sc}=38.07 mA/cm^2, FF=86.37%, η=28.07%}, the results showed that when the defect density of the Absorbent Layer varied from (1×10^9cm^{-3}) to (1×10^{18} cm^{-3}) while keeping the other cell parameters unchanged, as well as the defect density for the rest of the layers of the solar cell، it was observed that cell parameters were significantly reduced at high defect densities. Also, the defect intensity was changed in each of the Window Layer and the Back Reflection Layer separately, while keeping the rest of the parameters in the other layers the same. The density of defects in the interlayer was also changed while fixing the rest of the parameters, and the results were similar to what we obtained in the Absorption Layer, where with high concentrations of defects the cell parameters decrease significantly.**

Keywords: SCAPS-1D; CdTe solar cells; Defect Density in Solar Cell; (C-V) curve.

I. INTRODUCTION

Solar cells are photovoltaic devices that convert electromagnetic radiation from the sun into a continuous electric current [M. Lutfie., 2007].This enables us to obtain usable electrical energy from sunlight, as the light falling on it can penetrate into the p-n junction and transform into electrical energy [Ramprasaol C., 2012].This enables us to obtain usable electrical energy from sunlight, as the light falling on it can penetrate into the p-n junction and transform into electrical energy [S. M. Sze and K. N. G. Kwok, 2007].

Solar cells are used in terrestrial and space applications, as they are an important source for supplying the earth's satellites with the electrical energy they need. It is a candidate to be a strong potential alternative to terrestrial energy sources due to its good conversion efficiency and low cost when converting solar energy into electrical energy, as well as for not causing pollution [A.s Grove, 1997 and AL-Azawi, Maryam., 2014].

The year 1941 witnessed the manufacture of the first silicon cell with an efficiency not exceeding 1%, and in 1954 the American Bell Laboratories succeeded in manufacturing a silicon cell with an efficiency of 4%, with a thin layer thickness of 300 µm and a diameter of (3-6) cm and it was a single crystal of n-type or p-type with two metal electrodes made of Ti-Ag material, one connected to the front surface and the other to the back surface [S. M. Sze and K. N. G. Kwok,2007 and AL-Azawi, 2014].

Cadmium Telluride (CdTe) is used in thin film technology due to its high light absorption. It is also the second most widely used material in solar cells, after silicon. It crystallizes in the form of a Zinc Buckle (ZB), which is a compound with high stability and a high melting point 1365 K and its structural scheme is as shown in Figure 1. [Diso.D.G. (2011)].

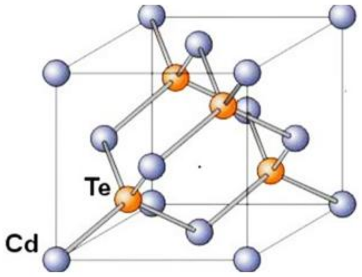

Figure 1: Structure composition of cadmium telluride

The semiconductor Cadmium Telluride is located in the periodic table (II-VI), and its direct optical energy gap is 1.45 eV, which is very close to the ideal energy gap for a solar cell [Adnan Hassan2021].

It is found in materials used in photovoltaic applications on a range of defects that vary between point defects of all kinds including vacancy, substitutional impurities and other linear defects, dislocations, micro defects, second stage deposits, surface defects and volumetric defects [B. Bagheri., 2020].

Defects in a solar cell can greatly reduce it's efficiency, therefore identification of these defects is critical, and defect detection is a necessary step towards improving the efficiency of the device. The defect must be linked to the performance of the solar cells and its impact on their work, so it is necessary to work to mitigate the defect or remove it, but working on treatment to remove the defect without harming the performance of the device in another way is not an easy matter, it is important to take the initial steps to identify the defects in the layers of the cell solar. There are three types of point defects:

1) Vacancies - missing atom of the lattice.
2) Interstitials - resulting from adding an atom between the regular lattice sites.
3) Substitutions - an atom that occupies the website of another element [V. Budhraja., 2012].

II. MATERIALS AND RESEARCH METHODS

SCAPIS-1D (Solar cell capacitance simulator) is a software program designed to simulate thin-film photovoltaic systems from the University of Gent in Belgium. [Rasha F. Hassan, 2020]. The program can be downloaded for free from the Internet, send a report to (Marc. Burgelman @ elis.ugent.be) and when the SCAPS version is downloaded, you will be asked to write down your name and the name of your organization.

This simulator enables us to study solar cells under conditions determined by the researcher. Using this program, we can describe a solar cell consisting of a maximum of seven layers and saves us the time and money needed to find the desired results from the solar cell by changing the thickness or type of layers and changing the percentage of impurities in it. He can solve semiconductor equations as Continuity equation and Poisson equation using Newton-Raphson method and density (electrons and holes) as well as drift and scattering equations and these equations control the behavior of semiconductors and we will summarize these equations as follows:

Drift and diffusion equation for electrons and holes

The total current density of the gaps in the semiconductor is called the sum of the components of the Drift current and Diffusion current of the gaps, as well as the total current density of electrons in the semiconductor as the sum of the components of the drift current and the diffusion current of the electrons. These equations can be summarized by the following relationships [Amu, Tochukwu Loreta., 2014].

$$Jn = q\ \mu_n\ nE + q\ Dn \frac{dN}{dX} \quad \text{.....................} \ (1)$$

$$Jp = q\ \mu_p\ pE + q\ Dp \frac{dN}{dX} \quad \text{.....................} \ (2)$$

Where Dn, Dp are constants called the Diffusion coefficients for electrons and holes, respectively, and μn, μp are the dynamics of the electrons and holes.

The mobility of Electron's and Hole's ($cm^2/V.s$).
Jn, Jp is the current density of electrons and holes.
The Electron's and Hole's current density (mA/cm^3).

Poisson's Equation

It is a relationship between the potential of electrons and the density of charges using Maxwell's equations (ΔD=p) and (D= ∈E) and the relationship between the electric field and voltage ($D(x) = -\frac{d\varphi(x)}{dX}$) [Rasha F. Hassan., 2020].

$$\frac{d\ ln(E(x))}{dx} . \frac{d\varphi\ (x)}{dx} + \frac{d^2\varphi}{dx^2} = \frac{f(x)}{\in(x)} \text{.....................} \ (3)$$

If (∈) is held constant, the Poisson equation is of the following form

$$\frac{d^2\varphi}{dx^2} = \frac{f(x)}{\in} \text{..........................} \ (4)$$

Continuity equation

This equation describes the change in the number of charge carriers for the reasons (Generation - Recombination) of the electron-gap pairs and that any action that happens to the charge carriers will lead to a change in the concentration of charge carriers. Continuity of electrons is in the form:

$$\frac{dn\ (x)}{dt} = Gn(x) - Rn(x) \text{ ....} \ (5)$$

The continuity equation for the gaps is:

Where Gn(x) represents the Generation of electrons, Rn(x) is the Recombination rate,

$$\frac{dp\ (x)}{dt} = Gp\ (x) - Rp\ (x) \quad \text{......................} \ (6)$$

The electric properties of the solar cell

Short Circuit Current Isc

It is the amount of current that flows in the solar cell when the circuit voltage = zero, which is the greatest current that the solar cell can give [Amu, Tochukwu Loreta., 2014].

$$I = I_o \left(\exp \frac{qv}{KT} - 1\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots (7)$$

Where I- Load circuit current, I_o- Diode saturation current,T- Temperature, K- Boltzmann constant

Open Circuit Voltage V_{oc}

It is the voltage between the metal ends of the cell when no current flows and it is the highest voltage that the solar cell can produce and is given by equation [13]:

$$V_{oc} = \frac{KT}{q} \ln \frac{Isc}{Io} + 1 \ldots\ldots\ldots\ldots\ldots\ldots\ldots (8)$$

Fill Factor FF%

It is the ratio between the output power of the cell divided by the open circuit voltage and the short circuit current (which together represent the ideal power for a solar cell) and is symbolized by FF[B. Bagheri, 2016].and it can be calculated by:

$$FF = \frac{V_m I_m}{Voc\ Isc} \ldots\ldots\ldots\ldots\ldots\ldots\ldots (9)$$

As for η, the efficiency of the solar cell is the ratio between the power generated by the solar cell and the power entering it from sunlight, if (PM) represents the maximum output power of the solar cell and represents (P_{rad}). The power entering it, which is the power of solar radiation, is taken as a rate of (1000 W/cm^2) [Hovel H. J. 1975].Calculated from the relationship:

$$\eta = \frac{P_m}{P_{rad}} \times 100\% \ldots\ldots\ldots\ldots\ldots\ldots\ldots (10)$$

It can also be found in the following form:

$$\eta = \frac{FF \times Isc \times Voc}{Pin} \ldots\ldots\ldots\ldots\ldots\ldots\ldots (11)$$

In our research, the cadmium telluride solar cell was selected, which is the solar cell consisting of five layers of absorption (CdTe), a permeable layer (CdS:O), a Buffer layer (Zn_2SnO_4) and a Transparent Conductive Oxide layer (FTO). And the Back reflection layer (Cu_2Te) shown in Figure 2. [Diso.D.G. (2011)].

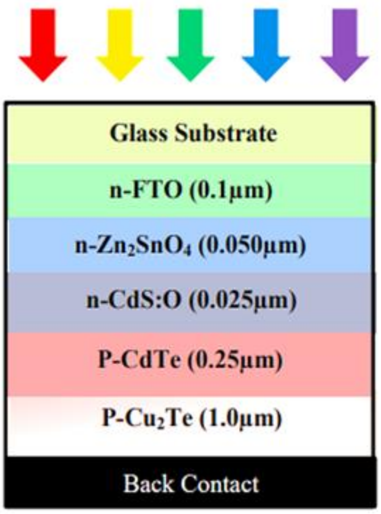

Figure 2: Certified solar cell structure

The concentrations of defects in our cell layers were as follows:

Absorption layer defect concentration (CdTe) at concentration [1×10^{10}cm^{-3}].

Focusing Defects of the window layer (Cds:O) at focus [1×10^{15} cm^{-3}].

Defect concentration of the reservoir layer (Zn_2SnO_4) at concentration [1×10^{15} cm^{-3}].

Concentration of the Transparent Conductive Oxide (FTO) layer at concentration [1×10^{15} cm^{-3}].

Back-reflection (Cu_2Te) layer focus when focusing [1×10^{10} cm^{-3}].

Using the parameters mentioned in the Tables in 1 and 2.[Matin. M.A., Amin, 2019، Matin, M.A., Tomal،Islam, A., Matin2019 and Chandrasekharan, r. (2012)].

Table 1: Parameters of solar cell layers

Parameter	p-Cu$_2$T$_e$	p-CdTe	n-CdS:O	n-Zn$_2$SnO$_4$	n-FTO
Thickness (μm)	1	0.25	0.025	0.05	0.1
Band gap (eV)	1.18	1.45	2.8	3.35	4.2
Electron affinity (eV)	4.2	4.28	4.5	4.5	4.5
Dielectric permittivity (relative)	10	9.4	1	9	10
CB. effective density of states (1/Cm^3)	7.80E+17	7.50E+17	2.20E+18	2.00E+18	1.20E+20
V.B. effective density of states (1/Cm^3)	1.60E+19	1.80E+19	1.80E+19	1.80E+19	7.00E+20
Electron thermal velocity(Cm/s)	1.00E+07	1.00E+07	1.00E+07	1.00E+07	1.00E+07

Hole thermal velocity (Cm/s)	1.00E+07	1.00E+07	1.00E+07	1.00E+07	1.00E+07
Electron Mobility (Cm^2/Vs)	5.00E+02	5.00E+02	1.00E+02	3.20E+01	2.00E+01
Hole Mobility (Cm^2/Vs)	1.00E+02	6.00E+01	2.50E+01	3.00E+00	1.00E+02
Shallow uniform donor density $N_D(1/Cm^3)$	0.00E+00	0.00E+00	1.00E+17	1.00E+19	1.00E+19
Shallow uniform acceptor density $N_A(1/Cm^3)$	1.00E+19	1.00E+15	0.00E+00	0.00E+00	0.00E+00
Defect type	single Acceptor	single Acceptor	single Donor	single Donor	single Donor
Capture cross section Electrons (Cm^2)	1.00E-12	1.00E-12	1.00E-17	1.00E-15	1.00E-15
Capture cross section Hole (Cm^2)	1.00E-15	1.00E-15	1.00E-15	1.00E-12	1.00E-12
Nt ($1/Cm^3$)	1.00E+10	1.00E+10	1.00E+15	1.00E+15	1.00E+15

Table 2: Parameters of interfaces of the simulation solar cell

Parameter	**n-Cds:O/p-CdTe**
Defect type	Neutral
Capture Cross Section Electron(cm^2)	$1X10^{-15}$
Capture Cross Section Hole (cm^2)	$1X10^{-15}$
Nt ($1/cm^3$)	$1X10^8$

III. RESULTS AND DISCUSSION

Effect of defect density in the CdTe Absorbent Layer

The CdTe Absorbent Layer absorbs photons from the sun with energy greater than the energy gap of the absorbing layer, in which results generated of electron-hole pairs. Finding some unavoidable defects in the solar cell materials, which leads to a decreased in overall performance of these cells.

We have been studied the defect density in the absorbent layer of CdTe on solar cell performance parameters over a wide range of defect density varying between(1×10^9 cm^{-3}) to (1×10^{18} cm^{-3}) and the defect level was set to 0.6 eV above the equivalence band while the other parameters remained unchanged such as the cross-sectional area of the pickup in the conduction layer which is equal to (1×10^{-15} cm^{-3}) as well as keeping the total density of defects in other layers the same, the results are shown in Figure 3.

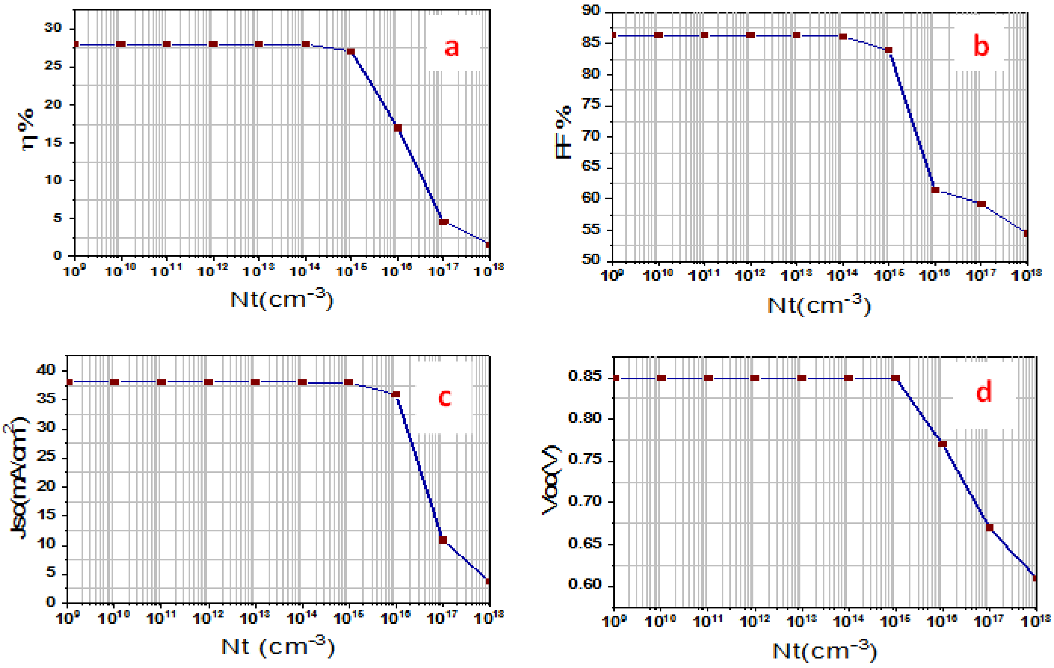

Figure 3: Effect of changing defect density in the absorber layer CdTe on solar cell parameters

From Figure 3-a, noticed that the conversion energy efficiency (η) decreased from 26.43% to 1.56% with changing of defect density from (1×10^{9} cm^{-3}) to (1×10^{18} cm^{-3}), noting that at concentrations less than 1×10^{14} cm^{-3} value of efficiency cell is almost constant, but at the density of defect1×10^{14} cm^{-3}, efficiency collapses sharply due to when the density of defects increased to a certain extent.

It causes an increased in the recombination rate of the electron-hole pairs, as well as an increase in the capturing processes. We also notice from Figure 3-b. that once the defect density increased from (1×10^{14} cm^{-3}), FF is reduced. Fast from (86.37%) to (54%), indicating losses in charge carriers.

Where capturing and recombination operations take place which becomes large while there was no change in FF value when defect density was less than (10^{14} cm^{-3}), on the other hand J_{sc} decreased rapidly from 38.07mA/cm^{2} to 3.73mA/cm^{2} once the defect density is exceeded (1×10^{15} cm^{-3}) noting that there is no change in the value of J_{sc} at the density of the defect is less than (1×10^{15} cm^{-3}) as shown in Figure 3-c.

We also notice from Figure 3-d. similar behavior for Voc, which decreased from 0.85V to 0.61V at The defect density varies from 1×10^{9} cm^{-3} to 1×10^{18} cm^{-3} with no noticeable change when the defect density is less than 10^{15} cm^{-3}.

We can deduced the high defect density from Figure 3.That it has a significant impact on the performance of the solar cell and that the explanation for this phenomenon is that the defect density affects the active layer is at the same time the absorbent region. It can be seen that with the increase in the density of defects, the lifetime of the charge carriers decreases and the recombination rate increases.

Effect of defection density in the Back Reflection layer (BSF)

To search for the effect of the defect density in the back reflection layer on the performance parameters of the solar cell, the defect density was changed from 1×10^{9} cm^{-3} to 1×10^{18} cm^{-3} and the defect level was set to be 0.6 eV above the valence beam where other parameters are set constant for all layers of the solar cell as shown in Figure 4.

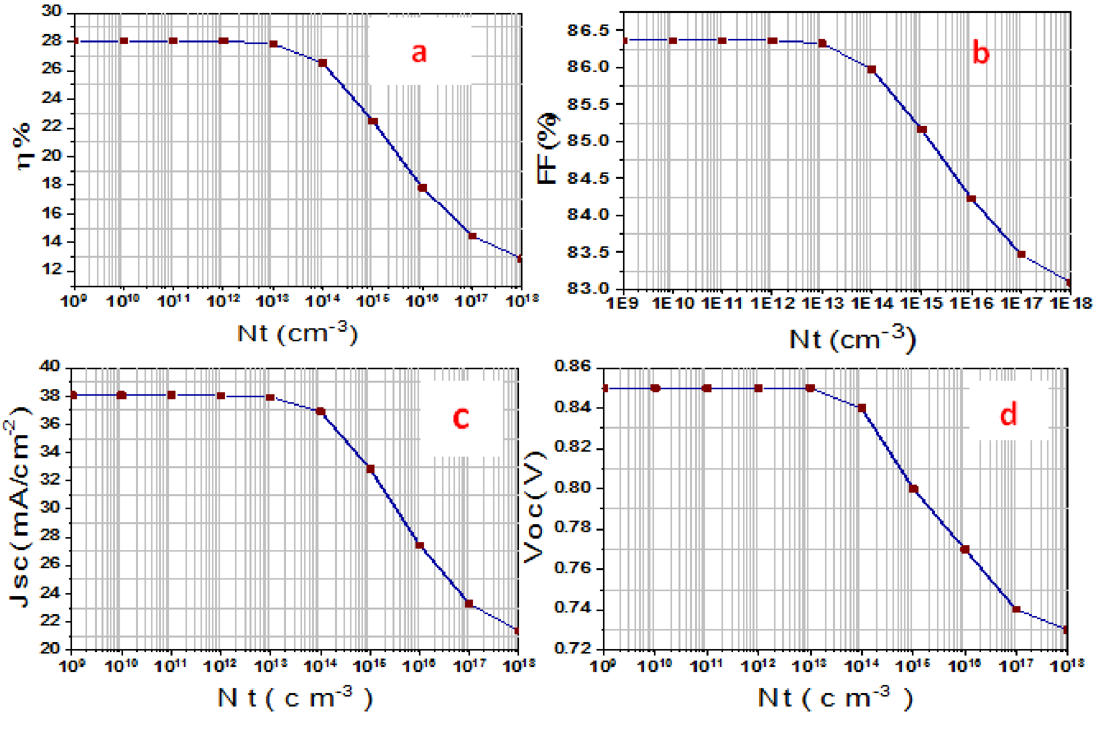

Figure 4: Effect of changing defect density in the back surface layer Cu_2Te on the solar cell parameter

Where we can notice from Figure 4-a. That the conversion efficiency energy (η)decreased from 28.07% to 12.9% with changing of defect density from 10^{9} cm^{-3} to 1×10^{18} cm^{-3}. Noting that at concentration of defects less than 1×10^{12} cm^{-3} the value of cell efficiency is almost constant but at the defect density 1×10^{12} cm^{-3} the cell efficiency starts to decline rapidly and also noted that once the defect density is higher than 10^{12} cm^{-3}, FF is rapidly reduced from 86.37% to 83.09% as shown in Figure 4-b, while there was no changing in FF when the defect density was less than 10^{12} cm^{-3}.

On the other hand, J_{sc} decreased from 38.07 mA/cm^2 to 21.36 mA/cm^2 when the defect density exceeded $1\times10^{13}1/cm^3$ while the value remained J_{sc} is stable at 38.07mA/cm^2 when the defect density is less than 1×10^{13} $1/cm^3$, while V_{oc} starts decreasing at the defect density greater than 10^{13} cm^{-3}, where it decreased from 0.85V to 0.73V and its value was fixed at 0.85V at the defect density less than $10^{13}cm^{-3}$ The reason is also due to increasing in the Recombination Rate of the electron-hole pairs at the high defects density in this layer.

Effect of defects density in Windows layer CdS:O

To find out the effect of changing the density of defects in the Windows layer CdS:O on parameters of solar cell, we changed the density of defects in this layer from 1×10^{13} $1/cm^3$ to 1×10^{22} $1/cm^3$ and the level was set the defect is to be 0.6 eV above the valence band level and the rest of the parameters of the other layers were kept the same and the results were as shown in Figure 5.

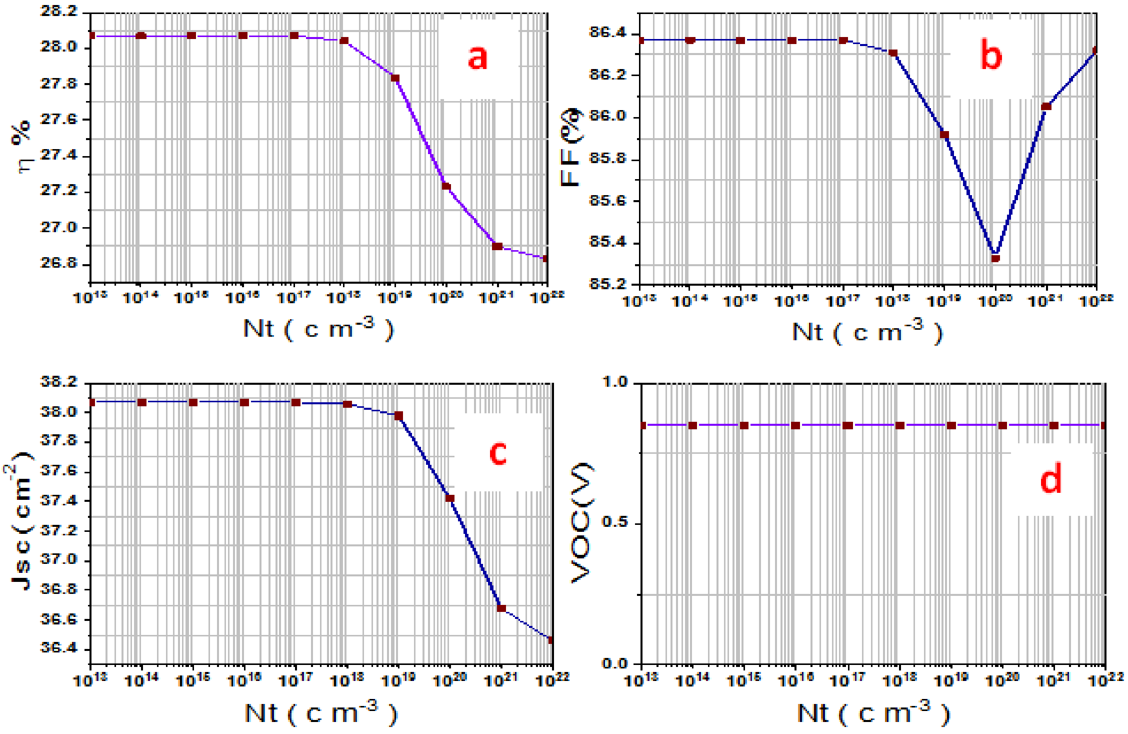

Figure 5: Effect of changing defect density in the Windows layer CdS:O on the solar cell parameter

It is noticed from Figure 5-a that the conversion energy efficiency (η) of the cell decreased from 28.07% to 26.83% when defects density of this layer changed From 1×10^{13} cm^{-3} to 1×10^{22} cm^{-3} and noted that at defects density less than 1×10^{17} cm^{-3} the efficiency of the cell is constant approximately when the defects density was greater than 1×10^{17} cm^{-3}, the efficiency of the cell began to decreased due to increasing in the electron-hole pairs Recombination Process. For Fill factor FF, it is observed that in the defect density range 1×10^{13} cm^{-3} up to 1×10^{17} cm^{-3}. There was no changing in its value but from the defect density 1×10^{17} cm^{-3} up to the defect density 1×10^{20} cm^{-3} very small decreasing in value of Fill Factor is observed to increasing the Recombination Process, but after increasing the defect density from 1×10^{20} cm^{-3}, the rise in the value of FF is noticed again, and the reason for this is that the high impurity for Windows layer CdS:O, it reduces the resistance and thus increasing the value of FF. [Chandrasekharan, r. (2012)].

As for short circuit current Jsc, it is noted that it started to decreasing from 38.07mA/cm^2 to 36.43mA/cm^2 when changing the defect density from $1\times10^{13}1/cm^3$ to 1×10^{22} cm^{-3} where the value of J_{sc} was constant at the defect density less than 1×10^{17} cm^{-3} but after the defect density 1×10^{17} cm^{-3} the value of J_{sc} begins decreasing due to the increasing in the Recombination Process for the electron-hole pairs. As for V_{oc}, it is noted that its value is not affected with the change of defect density in the Windows layer CdS:O.

Effect of changing the defect density in both the Zn_2SnO_4 Buffer layer and the Transparent Conduction Oxide layer

To search the effect of the density of defects in each of the Buffer layer and the Transparent Conduction Oxide layer separately, the defect level was set to be 0.6 eV above the valence band, where the other parameters were set constant for all layers of solar cell. In these two layers, they have no effect on the performance of the solar cell, as shown in Figure 6.

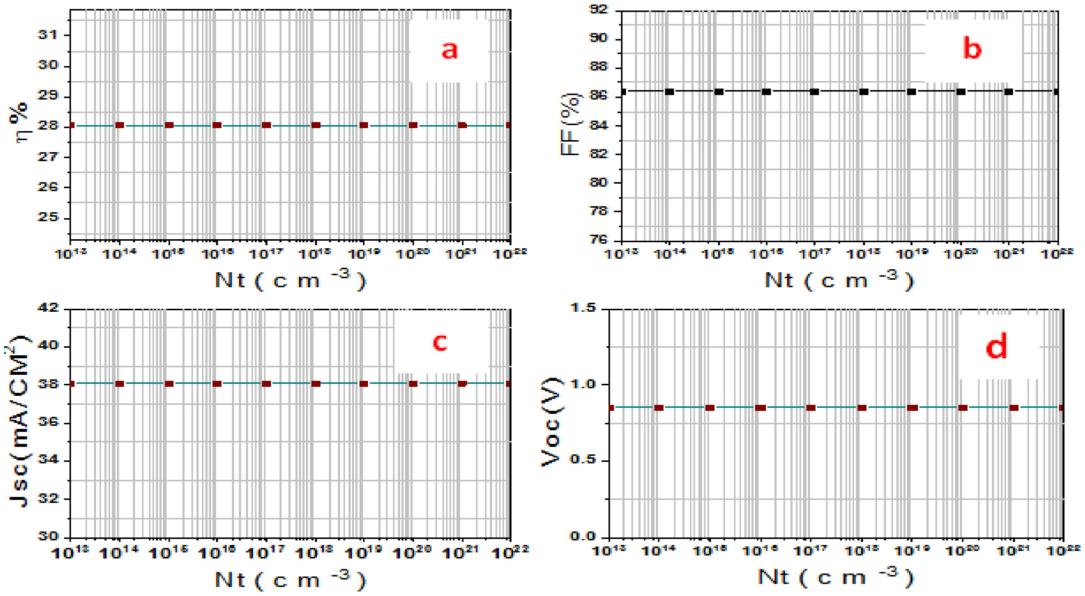

Figure 6: Effect of changing defect density in FTO and Zn_2So_4 on the solar cell parameter

To clarify this phenomenon, the role of these two layers is only to extract and transfer the holes and electrons from the Absorbance layer and not be affected by the difference in the density of the defect.

Effect of changing defect density in CdTe/Cds:O Interface layer on the parameters of solar cell

The effect of changing the defect density in the Interface layer on the performance parameters of solar cell was studied, as the defect density was changing from 1×10^7 cm^{-3} to 1×10^{15} cm^{-3} as shown in Figure 7.

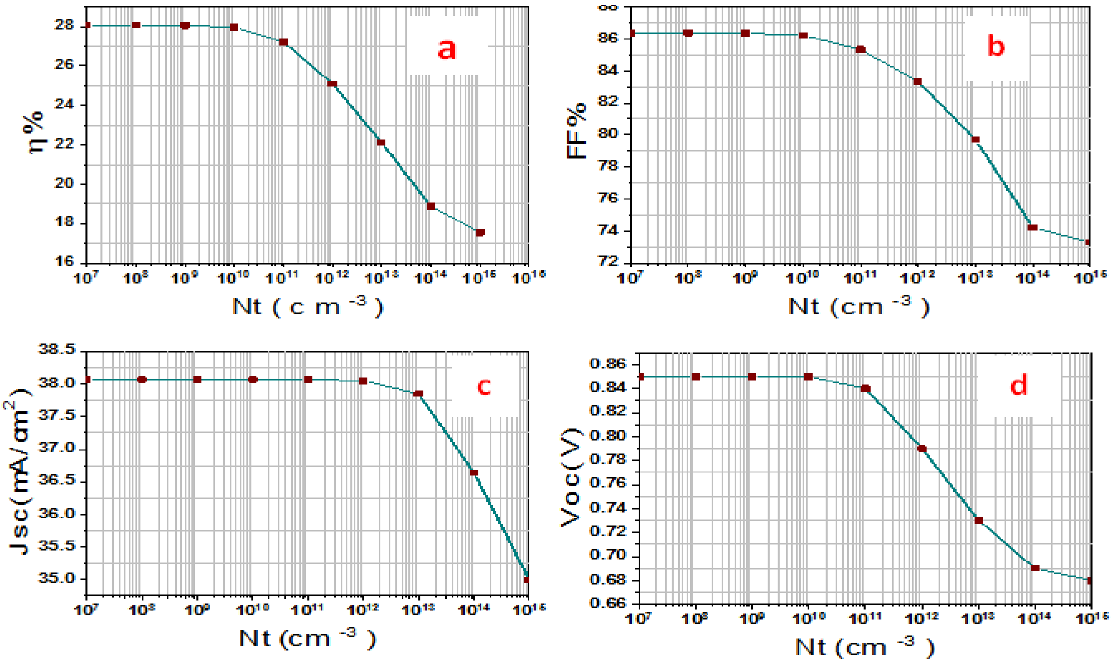

Figure 7: Effect of changing defect density in CdTe/CdS:O interface layer on the solar cell parameter

As can be seen in Figure 7-a, the efficiency of solar cell decreasing from 28.07% to 17.55% at this range of defects intensity and also preserved in its value. At the defect density less than 10^9 cm^{-3}, but after this density there was a decreasing in its value, that the Fill Factor FF exhibited a behavior similar to the conversion efficiency as it decreasing from 86.37% to 73.28% at the chosen range of change of defect density. Also, the effect of FF was not noticeable at the density of defects is less than 10^9 cm^{-3}, but after this density its value began decreased. As for J_{sc}, is noted that its value decreasing from 38.07 mA/cm^2 to $35A/cm^2$ when the defect density changed from 10^7 cm^{-3} to 10^{15} cm^{-3}, and as it was noticed in Figure 7-c that at the defect density less than 10^{11} cm^{-3}, the value of J_{sc} was almost constant but after this density, its value decreased. It is also noticed from Figure 8-d, that the value of V_{oc} decreasing from 0.85 V to 0.68 V when the defect density changed from 10^7 cm^{-3} to 10^{15} cm^{-3}, noting that there was no change at the defect density less than 10^{10} cm^{-3}, but at this concentration, the value of V_{oc} decreased significantly, and the reason is due to the influence of solar cell parameters at high defect densities also increase the Recombination Process of electron-hole pairs.

IV. CONCLUSIONS

Defects in the Absorber Layer and other layers of the interlayer in Cadmium Telluride (CdTe) cells are detrimental to their efficiency and stability, the present work will focus on investigating the effect of these defects on their electrical properties (I-V), this work was chosen to simulate solar cells using one-dimensional SCAPS-ID program.

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