Simulation Effect of Ga$_2$O$_3$ layer thickness on CdTe solar cell 
by SCAPS-1D.

Adnan Alwan Mouhammed, Ayed N. Saleh
Department of physics, Collage of Education for pure Science, Tikrit University, Tikrit, Iraq
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ABSTRACT

The effect of Ga$_2$O$_3$ thickness on CdTe cells was studied using the SCAPS-1D simulator. The best solar cell efficiency (14.65%) was found at the thickness of the gallium oxide layer (1-10nm) and the cell efficiency ($\eta$) decrease with an increase in the thickness of the oxide layer and the decrease of the fill factor, thus decreasing the voltage current (I-V) and decreasing the current of the short circuit (Isc). The value of the open circuit voltage (V$_{OC}$) is approximately constant and at 0.76V. The optical properties of the cell of quantitative efficiency are 86% and decrease within 18nm.

1- Introduction

A solar cell is a photovoltaic device made of a semiconductor material that converts sunlight into a direct current. In recent years, the study of binary compounds has increased in order to create new materials for solar cells. The researches has focused on thin-film solar cells for high efficiency at relatively low cost. Thin films made of column elements II-VI have been used in the periodic table in many semiconductor devices. In the periodic table, CdTe was one of the most promising materials in the production of thin films used in solar cells due to the energy gap of the solar cells. The CdTe solar cells are the most common kinds that dating to the 1952s and contain an ideal energy gap (1.45eV) for distribution of photon within the solar spectrum and high absorption coefficient ($5x10^5$ cm$^{-1}$) [1,2]. The efficiency of the cell in the 1990s reached 10% and researchers hope that the efficiency will reach 20%. Ga$_2$O$_3$ is a buffer due to the high band gap (4.7ev). It is a type n, which has been known for several decades. However, it has been increasingly used lately in the crystalline structure, which tends to be standard structure of semiconductors. It is similar to In$_2$O$_3$ and Al$_2$O$_3$, the GaN family and is used in the heterojunction system as well as homojunction. (Solar cell capacitance simulator) SCAPS-1D simulation program, a one-dimensional solar cell simulator program designed by the University of Gent [3] in Belgium, the original program for family structures (GaAs, Si) as well as non-crystalline ones. The objective of the study is to test the effect of Ga$_2$O$_3$ thickness on the performance of the CdTe solar cell and the study of both open-circuit voltages (Voc) Short circuit current (Isc), fill factor (FF), cell efficiency ($\eta$).

2. Theoretical model

The SCAPS-1D (a solar cell capacitance simulator) is one dimensional solar cell simulation program can solve basic semiconductor equations such as continuity equation, Poisson equation, carrier density, generation process, and recombination where the continuity equation for holes $\frac{\partial n(x)}{\partial t}$ and electrons $\frac{\partial n(x)}{\partial t}$ is given as follows: [4]

$$\frac{\partial n(x)}{\partial t} = G_n(x) - R_n(x) \ldots (1)$$

where $G_n$ represents the generation process for electrons and $R_n$ represents the recombination rate. The continues equation for holes given by the equation:

$$\frac{\partial p(x)}{\partial t} = G_p(x) - R_p(x) \ldots (2)$$
where $G_p$ represents the generation process for holes and $R_p$ represents the recombination rate. The charge density($\rho$) the potential($\phi$) and electron permittivity ($\varepsilon$) are related to the Poisson equation and the following formula [4]:

$$\frac{d}{dx} \left( \frac{1}{\varepsilon} \frac{d\phi(x)}{dx} \right) + \frac{d^2\phi}{dx^2} = -\frac{\rho(x)}{\varepsilon(x)} \quad \ldots (4)$$

If $\varepsilon$ is constant, the Poisson equation is in the following formula:

$$\frac{d^2\phi}{dx^2} = -\frac{\rho(x)}{\varepsilon} \quad \ldots (6)$$

The current passing through the solar cell is as follows:

$$I = I_0 \left( \exp \frac{q\phi}{kT} - 1 \right) - I_l \quad \ldots (7)$$

where $I$ is the current of the load, $I_l$ is the photocurrent, $I_0$ Reverse saturation current, $T$ the absolute temperature, $K$ is the Boltzmann constant and $\nu$ the load voltage which is equal to zero when the load resistance is zero, the current passing is the short circuit current, when the voltages equal zero, equation 7 becomes the following formula: [5]

$$I_{sc} = -I_l \quad \ldots (8)$$

Short circuit current (Isc) In the case of the open circuit voltage, the resistance is large as possible and the current is zero [5]

$$V_{oc} = \frac{kT}{q} \ln \left( \frac{I_0}{I_l} \right) + 1 \quad \ldots (9)$$

where $V_{oc}$ is the open circuit voltage, the fill factor is a measure of the reference range of the output properties and its value for the cells with acceptable efficiency between (70 -85) % and is defined according to the following relationship: [5]

$$FF = \frac{V_{oc}I_m}{V_{oc}I_{sc}} \quad \ldots (10)$$

where $V_m$ and $I_m$ are the maximum of the voltage and current respectively, the efficiency of solar cell can be write as [5]:

$$\eta = \frac{\text{output power}(P_m)}{\text{input power}(P_{in})} \times 100\%$$

$$\eta = \frac{I_mV_{oc}}{P_{in}} \times 100\% \quad \ldots (11)$$

Thus, equation (11) can be write as:

$$\eta = \frac{FF \times I_{oc} \times V_{oc}}{P_{in}} \times 100\% \quad (12)$$

3– Cell description

The solar cell we have studied is composed of (TCO / Ga$_2$O$_3$ / CdTe). The TCO represents the transparent metal oxides made from ZnO and has a higher transparency (85%) at wavelength (550nm) [2]. Gallium oxide is a substance high energy gap (4.7ev) and called a buffer layer [6]. CdTe is a semiconductor material with a band gap (1.45ev) as illustrated in fig 1. The defect for CdTe is an acceptor and for Ga$_2$O$_3$ a donor as shown in the table (1). Some defects create their own energy levels in the band gap of semiconductor [7], which results in formation of trapping centers for charge carriers (electrons and holes).

When the charge carriers capture on such centers, they either loose time before reaching the edge of semiconductor edges, or vanish due to recombination.

| TCO | Ga$_2$O$_3$ (1-30) nm | CdTe (5µm) | Back contact |
|---|---|---|---|
| Thickness | 1-30 nm | 5 µm | |
| Band gap | 4.8 eV | 1.45 Ev | |
| electron affinity (eV) | 3.5 | 4.3 | |
| Dielectric permittivity | 9.93 | 9.4 | |
| CB effective density of states (1/cm$^3$) | 2.2x10$^{18}$ | 1.3x10$^{19}$ | |
| VB effective density of states (1/cm$^3$) | 1.8x10$^{19}$ | 7.6x10$^{18}$ | |
| electron thermal velocity (cm/s) | 1x10$^7$ | 1x10$^7$ | |
| hole thermal velocity (cm/s) | 1x10$^7$ | 1x10$^7$ | |
| electron mobility (cm$^2$/Vs) | 10 | 50 | |
| hole mobility (cm$^2$/Vs) | 10 | 30 | |
| shallow uniform donor density ND (1/cm$^3$) | 2x10$^{15}$ | 0 | |
| shallow uniform acceptor density NA (1/cm$^3$) | 10 | 1x10$^{13}$ | |
| T(k) | 300 | 300 | |
| Rs (Ω.cm$^2$) | 0.1 | 0.1 | |
| Defect type | Donor [8] | Acceptor [7] | |
| energetic distribution | Single | Single | |
| Nb total (1/cm$^3$) | 1x10$^{19}$ | 1x10$^{19}$ | |
| Capture cross section electrons (cm$^2$) | 1x10$^{-13}$ | 1x10$^{-13}$ | |
| Capture cross section hole (cm$^2$) | 1x10$^{-12}$ | 1x10$^{-10}$ | |

Fig. 1: Installation of solar cell used in research


4–Results and discussion

4-1 Effect of Ga$_2$O$_3$ on I-V Properties

Photocurrent is one of the most important parameters affecting the efficiency of the solar cell. The general formula of these curves is a rise in the value of the current with increasing width of the depletion region, which increases built in potential. Thus, the probability of electron-holes separating is increased and reduces the recombination process on the interface, which increases the photocurrent [9]. When the thickness (5,10) nm of the recombination on the interface is very weak, the effect of the Ga$_2$O$_3$ on the I-V properties causing a reduction in the voltage-current curve with increase in the thickness of the buffer layer. We studied a voltage current at the thickness of (5,10,15,20,25,30) nm as shown in figure (2A).

The decrease in(I-V) curve is with on increase in the thickness is due to reduction in photo current. Increasing the thickness increases the process of the recombination on the interface [5], so that the rate of generation of electron-hole will be pair reducing short current (Isc), because formation of trapping centers Which works to depletion hole will be pair reduction in the fourth quarter and decreasing the fill factor. The photovoltaic cell is as good as the fill factor about one, the effect of oxide thickness on fill factor illustrated in figure (3A). In this figure, we find three regions, the first region (1-10nm), where the fill factor reaches 82% and don’t exceed 85% because the absorbance of TCO layer [11]. The second region, when the thickness of (10-23) nm shows a linear decline, until (78%) at the thickness of (10nm) and reach (5%) at the thickness of (23nm) because recombination at interface, thus causing to capture electrons and reduce the current [12]. While the third region at (23nm) and above, the fill factor is reduced to its lowest value. This is due to the fact that the fill factor is affected by increasing the series resistance [12]. The higher thickness of the gallium oxide, lead to higher of the series resistance and the decreasing in fill factor. The effect of gallium oxide on open voltage circuit is slight. The increase in the thickness of the gallium oxide leads to a reduction in the photocurrent, which is linearly linked to the voltage open circuit, resulting in lower open circuit voltages but slightly [10]as show in figure (3B).

The efficiency of the solar cell is defined as the ratio between the output power of the solar cell and the power incident on it. As the increase in the thickness of the gallium oxide layer has a negative effect on each of the above electrical properties. The increase of the thickness decreases the short circuit current (Isc), the open voltage circuit (Voc) Fill Factor and efficiency of the cell decreases with increasing the thickness of the gallium oxide, as shown in figure (4).

We find that the efficiency of the solar cell is constant with the increase of thickness up to (9nm) and then decreases with the increase of thickness above the that because the density of electrons is high within this range and then show linear decrease with thickness due to centers of the recombination at the interface, which affects the value of efficiency.

![Fig. 2: Effect of Ga$_2$O$_3$ layer thickness on A(V-I) curve, B -Short Circuit Current (Isc)](image)

![Fig. 3: Effect of Ga$_2$O$_3$ on the, A (Fill Factor (FF)), B (voltage open circuit(Voc)).](image)
4.1.2 Effect of Ga$_2$O$_3$ on C-V Properties and band diagram

The characteristics of the C-V are important electrical properties that calculate the width of depletion($V_{bi}$) determine the type of junction whether it is Abrupt or Graded. Increasing the thickness increases the value of the capacitance and therefore reduce the amount of depletion layer as in the figure (5A). As the increase in fish work to change the difference among Fermi level and the level (En) conduction band (Ec) and Fermi level(Ep) and level band (Ev), which increases the process of depletion as in figure (6) (A,B,C,D,E,F). It is noted that the oxide region is completely depleted, especially with positive voltages. In the negative voltages, the total depletion region is shown in CdTe and the relationship between the capacitance and the depletion area as follows:

\[ C = \frac{\Delta Q}{\Delta V} = \frac{\Delta \omega}{\omega} \quad (13) \]

Where dQ changes the charge of the depletion layer, dV the applied voltage \( \omega \) width of the depletion region and as in figure (5B).

Fig. 4: shows the effect of Ga$_2$O$_3$ on cell efficiency ($\eta$)

Fig. 5: Effect of the thickness of the Ga$_2$O$_3$ layer on the. A (depletion layer (W)), B(C-V Properties)
4.1.3 Effect of Ga$_2$O$_3$ on Quantum Efficiency (QE)

Quantum efficiency is an important optical factor in solar cells, and QE is defined as the number of electron-hole pairs generated by incident photon [15]. The increase of Ga$_2$O$_3$ thickness layer increase affects the performance of the solar cell and thus affects absorption cell and reduce the efficiency of the solar cell see figure (8). The highest value of the quantitative efficiency is about (85%), Within the wavelength (300-825) nm at thickness (1-18) nm and then the quantum efficiency decreases because the increase in the absorption of photons from the Ga$_2$O$_3$. 

The figure (7) shows a larger part of the previous forms. The increase in thickness shows the high of Fermi level and increases the capacity of the cell.

**Fig. 6:** Effect of the thickness of the Ga$_2$O$_3$ oxide layer (A=5nm, B=10nm, C=15nm, D=20nm, E=25nm, F=30nm) on the Energy band.

**Fig. 7:** Larger shape of energy band
oxide layer, which reduces the rate of generating pairs, which affects the value of quantum efficiency [16]. At wavelength greater than λ = 825nm where the process of absorption of cadmium Telluride (CdTe) occurs as shown in figure (8).

Figure 9 shows that the best thickness of gallium oxide is about (1-18) nm, which has a high quantum efficiency at wavelength (550nm).

5. Conclusions

we have found that increasing the thickness of the buffer layer significantly affect the properties of the current - voltage because of the recombination increased at the interface. The best thickness of the buffer layer is up to (1-10) nm and increase the thickness are very effective on short circuit, fill factor as well as the impact of the efficiency of the cell.

Increasing the thickness of the oxide layer affects the properties of the capacitance - voltage and Increasing the thickness of the oxide layer reduces the depletion layer, which increases the capacitance of the cell. The optical properties found that increasing the thickness of the oxide layer works to reduce the absorption of incident photons and thus reduce the quantum efficiency.

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محاكاة تأثير سمك طبقة أوكسيد الكالسيوم الثلاثي على خلايا تيلورايد كادميوم الشمسية باستخدام SCAPS-1D

عبدان علوان محمد عبدالله، عادل نجم صالح
قسم الفيزياء، كلية التربية للعلوم المصرفية، جامعة تكريت، تكريت، العراق

الملخص

تم دراسة تأثير سمك طبقة الحاجز Ga2O3 على خلايا تيلورايد الكادميوم CdTe باستخدام محاكى SCAPS-1D. وجد أن أفضل كفاءة للخلايا (14.65%) عند سمك طبقة الحاجز تتراوح (1-10nm) بانخفاض مع زيادة سمك طبقة الاوكسيد Gao3. وتتىك كفاءة الدائرة (I-V) وانخفاض منحنى تيار - جهد (I=V) وفق ذلك تيار الدائرة القصير (Isc). أما قيمة فولتية الدائرة المفتوحة (Voc) ثابتة تقريبا وبحدود (0.76V). أما الخواص البصرية للخلايا المتمثلة بالكفاءة الكمية تكون كيمتها (86%) وتتىك ضمن سمك (18nm).