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DESIGN AND SIMULATION OF AN EFFICIENT SOLAR CELL WITH SB_2SE_3 AND CDTE AS DOUBLE ABSORBER LAYERS

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Abstract. *The present study proposes a solar cell using double absorber layers of Sb_2Se_3 and CdTe. The design aim is to obtain high efficiency while maintaining or improving other main characteristics of solar cell. The proposed Sb_2Se_3/CdTe/CdS/ZnO/SnO_2 solar cell include additional Sb_2Se_3 layer compared with its conventional counterpart while their total thickness is equal. The SCAPS simulator software has been applied to investigate the device performance. Firstly, the impacts of applying two absorber layers on the cell's performance and their thickness ratio were studied. Then, the effect of limitations such as band gap energy and the impurity concentration of the Sb_2Se_3 layer, the work function of the back contact metal, and the operating temperature on the cell performance were investigated. For thickness of 1.3 µm of Sb_2Se_3 layer and 0.7 µm of CdTe layer, the efficiency of 32.40% was obtained. The short circuit current density is J_{SC}=34.55 mA/cm^2, the open circuit voltage V_{oc} = 1.06 V, and the Fill Factor is FF = 86.06%. The obtained efficiency is about 5% higher than the structure where only the layer of CdTe is applied as the absorber. Also, the use of Te which is a limited supply material in environment is reduced in proposed structure. Simulation results demonstrate that a solar cell with higher efficiency and more compatible with environment can be achieved using the proposed two absorber layer.*

Key words: *solar cell, double absorber layers, Sb_2Se_3 layer, efficiency, fill factor*

1. INTRODUCTION

In the last few decades, the research community witnessed the noteworthy advancement in the field of solar photovoltaic technology (PV). Many groups of solar cells including copper indium gallium selenide (CIGS), perovskite cells, cadmium telluride (CdTe), silicon, and cells based on semiconductor compound III and V have been considered to make more

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competent cells. The thin film CdTe and CIGS based cells as 2[nd] generation of solar cells present a proper coefficient of absorption in the visible range of spectrum. Sb_2Se_3 (antimony selenide) is also an appropriate absorber material in photovoltaic applications. Its band gap is direct in the variety of 1.2-1.9 and 1-1/5 eV, related to the deposition methods and operating circumstances. However, there are few reports on applying Sb_2Se_3 as the BSF (Back Surface Field) layer, in case of heavy doping of 10^{20} cm^{-3} [1].

Silicon-based solar cells are efficient cells whose manufacturing techniques are complex and expensive. Reasonable cost third-generation thin-layer solar cells have been evaluated as a potential substitute to monocrystalline silicon (Si) counterparts. The thin layer cells based on a-Si (amorphous silicon), CIGS, and CdTe, have been studied as fruitful structures. The CdTe technology is cheaper than others, 30 percent and 40 percent cheaper than CIGS and a-Si technology, respectively. Thus, the CdTe based cells show higher ratio of efficiency/cost.

The polymer and perovskite-based cells have attracted the attention of researcher in recent years. The problem is that these solar cells are unstable, which limits their long-term applications [2]. On the other hand, it is not yet considered for large-scale application because compounds such as lead (Pb) are harmful to human health and biological life. Thin-layer photovoltaics have received more attention. It is due to the use of fewer materials, processing methods with low-temperature, variability of deposition procedures, well-matched with low-cost platforms, and low manufacturing expenses. Thin layer cells based on copper indium di-selenide, CdTe, and CIGS have now reached the commercialization step. But, factors such as the limited supply of Te and In due to scarcity, the Cd toxicity, and expensive price of Ga have made worries about the restrictions in PV manufacturing volume. Additional absorber substances in thin film cells have been considered, such as SnS (tin sulphide), FeS_2 (iron sulfide), Cu_2O (copper oxide), Cu_2S (copper sulfide). However, the conversion efficiency obtained from these materials is still much lower than expected. Among all adsorbents, Sb_2Se_3 is a single-phase, stable, and binary chalcogenide compound [3,4].

CdTe thin-film structures have proven to be competent and gainful in generating solar electricity. They are competitor for CIGS and SI wafers in the commercial photovoltaic market. Significant study consideration has been dedicated to growing the conversion efficiency of these cells, so that has touched 22%. The CdTe efficiency does not depreciate at high temperatures due to its proper stability both chemically and thermally. On the other hand, CdTe has high chemical and thermal stability, which is caused by the large binding energy between Te and Cd (5.75ev). This is far larger than any energy of photons in the solar spectrum. Consequently, cell destruction and the existence of toxic cadmium is not a severe problem in environmental claims. A method to reduce the contest of Te deficiency is to decrease the CdTe thickness, where the normal CdTe thickness is presently about 5 µm. By reducing the thickness, not having significantly reduction in its proficiency, the amount of materials and its cost will also be reduced [5].

In this work, the thickness of the CdTe is considered to be very thin, which leads to less consumption of Te, and because of the less use of toxic Cd, it is better compatible with the environment. To compensate for the decrease in solar cell efficiency caused by the decrease in the thickness of absorber, another material has been used as the second absorber layer. CdTe is one of group II and VI combined polycrystalline semiconductors, with about 1.5eV direct band gap beside considerable absorption coefficient (1×10^5 cm^{-1}). In recent years, the application of CdTe in the field of thin film solar cells with high efficiency has been significantly developed. Related to long-standing stability, inexpensive manufacturing of solar cells, and capability of absorbing wavelengths between 350 and 850nm, their production seems promising [6]. Researchers have formerly confirmed efficiency of 18.7% in polycrystalline thin-film CdTe cells. It achieved by means of higher deposition temperatures, back-contact Te layers, and anti-reflective coating [7]. The recombination at the back contact interface can be reduced by using a back contact field layer in CdTe cells, leading to improved open circuit voltage (V_{oc}). By using a NiO layer in the back contact, Di Xiao and colleagues succeeded in making a CdTe-based structure with 12.17% efficiency and V_{oc} of 790mV [8]. Moreover, in 2021, Rahmand and colleagues planned a CdTe-based solar cell in which antimony sulfide was used for the first time as the HTL (hole transport layer) at the back surface field [9]. They reached an efficiency of 28.41%.

The Sb_2Se_3 with hole mobility up to 42 $cm^2v^{-1}s^{-1}$, as a semiconductor is p-type with an orthogonal crystal structure. Its absorption coefficient is high. In addition, Se and Sb are relatively abundant, inexpensive, and less toxic. In 2018, researchers used vapor transfer deposition (VTD) method to Sb_2Se_3 film deposition laterally in the orientation of 221 type to increase the efficiency equal to 7.6%. Li and colleagues, in 2019 also employed the close-spacing sublimation method to effectively raise Sb_2Se_3 nanorod arrays with 001orientation on a Mo electrode [10]. They obtained the maximum yield about 9.2% to date. The V_{oc} and short circuit current density (J_{sc}) of Sb_2Se_3 solar cells are far from ideal, in spite of such quick advance. To extra progress in the performance of the device, many limitations require to be examined, which leads to a huge burden on experimental study [10].

This study has theoretically investigated the effect of applying two absorber layers of Sb_2Se_3 and CdTe, as well as the role of changed limitations on solar cell outputs. To evaluate the output of the proposed cell, SCAPS simulator has been used. SCAPS is able to obtain the outputs of the related semiconductor equations; Poisson and carriers continuity equations. SCAPS calculates the answer of the straightforward semiconductor equations in one-dimensional and stable circumstances [11].

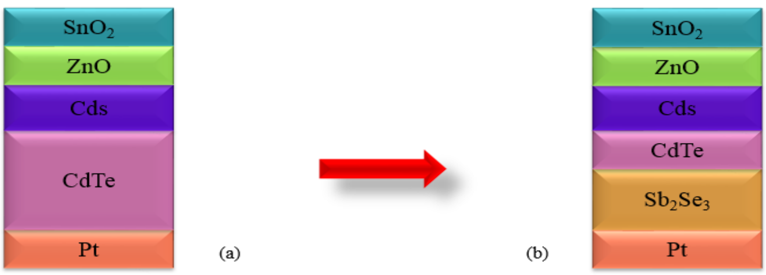

Fig. 1 Representation the construction of (a) the basic and (b) the proposed Sb_2Se_3 / CdTe solar cells

2. Simulation of Projected Solar Cell

2.1. Cell Construction

Figure (1) presents the schematic construction of a CdTe-based and the proposed cell with two absorber layers. Sb_2Se_3 and CdTe are the absorber layers. The thickness of absorber layer is more than the other layers, so it allows more sunlight to be absorbed in this layer [12]. CdS, which has a high absorption coefficient, appropriate ohmic contact, and low resistance, has been used in the buffer layer. SnO_2 is chosen as TCO (transparent conductive oxide) and ZnO as high resistivity transparent (HRT) layer. Also, platinum is applied as the back contact metal. It should be mentioned that the thickness for Sb_2Se_3 and CdTe of proposed cell mentioned in figure is selected such that the cell characteristics obtain the proper values where it will be discussed in other sections.

Table 1 Input parameters of SCAPS 1-D to simulate the device performance

Parameters	SnO_2	Zno	CdS	CdTe	Sb_2Se_3
Electron affinity (eV)	4.0	4.0	4.0	3.9	3.9
Mobility of Electron (cm^2/V_S)	100	25	100	320	15
Mobility of hole (cm^2/V_S)	25	25	25	40	5.1
Electron thermal velocity (cm/s)	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
Thickness (µm)	0.05	0.05	0.06	0.7	1.3
VB effective density of states (cm^{-3})	1.8×10^{19}	2.4×10^{18}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
CB effective density of states (cm^{-3})	2.2×10^{18}	1.8×10^{19}	2.2×10^{18}	8×10^{17}	2.2×10^{18}
Hole thermal velocity (cm/s)	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
Acceptor density N_A (cm^{-3})	0	0	0	1×10^{14}	1×10^{18}
Donor density N_D (cm^{-3})	1×10^{17}	1×10^{19}	1×10^{18}	0	0
Bandgap (ev)	3.6	3.37	2.4	1.5	1.33
Dielectric Permittivity	9	9	10	9.4	18
Defect type	Donor	-	Neutral	Donor	Neutral
N_t total (cm^{-1})	1×10^{15}	-	1×10^{14}	1×10^{13}	1×10^{12}
Energy level related to a reference (eV)	1.8	-	0.6	0.75	0.6
Energetic Distribution	Gaussian	-	Single	Gaussian	Single
Reference for defect energy level E_t	midgap	-	Above EV	midgap	Above EV
Holes capture Cross-Section (cm^2)	10^{-15}	-	10^{-15}	10^{-15}	10^{-15}
Electron capture Cross-Section (cm^2)	10^{-12}	-	10^{-15}	10^{-12}	10^{-15}

2.2. Parameters of Simulation

The characteristics of the proposed Sb_2Se_3/CdTe/CdS/ZnO/SnO_2 cell have been extracted from the [13, 14, 15, 16] references, and they are outlined in Table (1). The defect energy distribution of CdTe and SnO_2 is Gaussian with a characteristic energy of 0.1eV [13]. Also, the defect of the interface is also collected from reference [1] and summarized in table (2).

Table 2 Interface defect characteristics

Parameter	CdS/CdTe interface	Sb_2Se_3 CdTe interf
Defect type	Neutral	Neural
Total density (cm^{-2})	1.0×10^{14}	1.0×10^{14}
The energy related to Reference (eV)	0.25	0.25
Reference for defect energy level Et	Above highest Ev	Above highest Ev
Holes/Electrons capture cross section (cm^2)	1×10^{-19}	1×10^{-19}

3. Discussion and Results

The current work aimed to design a solar cell with high efficiency and simultaneously more compatibility with the environment. Here, a 2 µm thickness CdTe-based solar cell was first simulated as the only absorber layer. Then, the CdTe thickness has been decreased. It is more economical since it applies less Te that is less abundant, and more compatible with the environment due to the less usage of the toxic Cd. However, by reducing the thickness of the CdTe layer, the efficiency experiences a reduction, as depicted in Figure 2. It should be mentioned that between 1 µm and 2 µm, the efficiency experiences small changes (about 1%). Here the thickness of basic structure is selected to be 2 µm but one can choose a thickness between 1 µm and 2 µm without losing considerable efficiency. In Figure 2, the solar cell includes only one absorber layer. In next simulations, the second absorber layer is inserted but the total thickness of absorber layers (CdTe/Sb_2Se_3) is 2µm. To evaluate the effect of using two absorber layers, firstly, the total 2µm thickness is devoted to Cd and then the effects of reducing the CdTe thickness and increasing Sb_2Se_3 have been investigated.

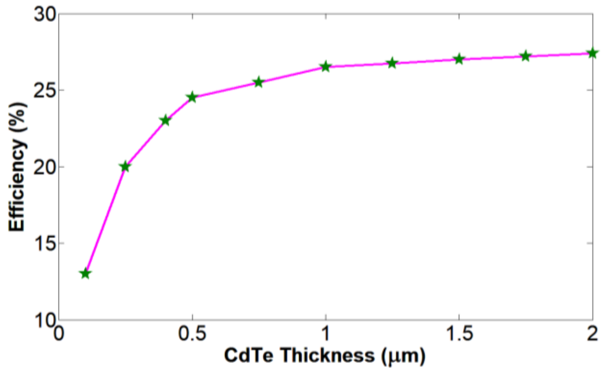

Fig. 2 Influence of reducing the CdTe absorber thickness on efficiency

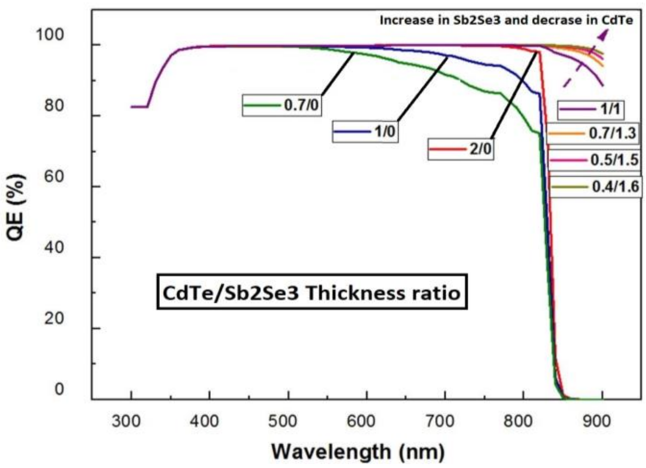

Fig. 3 The consequence of reducing the CdTe layer thickness and using two absorber layers on the QE of the structure. By increasing the Sb_2Se_3 thickness, the QE increases

Figure 3, presents the cell quantum efficiency (QE). The decrease in efficiency is due to the decrease in QE for the wavelengths greater than 500 nm. For one absorber layer the QE is zero for wavelength greater than 850 nm. By adding second absorber layer, which is placed at the front of the cell, the decrease in solar cell efficiency is compensated. Sb_2Se_3 has well abundance and less toxicity, and depending on the deposition methods, can have a direct band gap in the variety of 1-1.5 eV, and considering that its energy is less than CdTe in this range, this material is chosen to be the second absorber layer. The effect of its application on quantum efficiency is revealed in Figure 3. As it is given in the figure, if CdTe is used as the only absorber layer, the quantum efficiency will be zero for the photons with a wavelength longer than 850nm. By applying Sb_2Se_3 as the second absorber layer, the cell would be able to absorb photons with longer than 850nm wavelength, and due to absorbing more photons, the cell's efficiency improves. It was observed from Figure 3 that by applying two absorber layers with different band gap energy, the cell absorbs more extensive solar energy, which increases the cell's efficiency.

In subsequent, the effects of thickness ratio of the absorber layers, the Sb_2Se_3 band gap energy, temperature, etc., on the characteristics of the structure including V_{oc}, J_{sc}, FF, and efficiency (η) are examined. The efficiency and FF of the solar cell can be calculated by means of the bellow relations [17], where P_{in} is input power, V_m and I_m are maximum values of voltage and current, respectively.

$$\eta = \frac{I_{SC}.V_{OC}.FF}{P_{in}}, \quad (P_{in} = 1000\ \frac{w}{m^2}) \tag{1}$$

$$FF = \frac{I_m \times V_m}{I_{SC} \times V_{OC}} \tag{2}$$

3.1. Examination of the Thickness Ratio of the Sb_2Se_3 and CdTe and the Effect of Using Two Different Absorber Layers

The absorber thickness is a significant restriction that affects the capabilities of the solar cell. A thick layer permits further photons to be absorbed, thus producing further electron-hole pairs and improving proficiency. Because of weak optical absorption, a thin absorber layer reduces the optical current, thus the efficiency. In another word, if the absorber layer is too thick, it will lead to a longer transmission path of the optically produced carriers; thus, the recombination increases. Also, there is an optimal thickness for the absorber layer beyond which the output parameters do not improve significantly. In this work, the thickness ratio of the two absorber layers has been changed. Table 3 displays the thickness ratio of the two absorbers, and Figure 4 presents the output characteristics of the solar cell concerning these thicknesses.

Table 3 Several thickness ratio of CdTe and Sb_2Se_3 absorber layers

Structure	A1	A2	A3	A4	A5	A6	A7
CdTe/Sb_2Se_3 Thickness (μm)	2/0	1.7/0.3	1.3/0.7	1/	0.7/1.3	0.5/1.5	1/1.9

As seen in Figure 4, η, J_{SC}, and FF are greater when the absorber layer is composed of two different types of material than the state where it is only constituted of one type of material. Therefore, the efficiency can be improved by applying double absorber layers, which is due to the absorption of a wider range of solar energy. Consequently, FF will also be improved according to the relation (2). According to Figure 4, the utmost V_{oc} corresponds to (A_1) that only the CdTe absorber layer has been used, and it caused by the decrease in the back surface field recombination. Yet, the short circuit current in this state is less than in the other states.

In the case of the thickness ratio of 0.7/1.3 of the CdTe/Sb_2Se_3 absorber, the efficiency of the solar cell has amplified by 5% related to the first state where only one layer with the thickness equal to 2 µm was applied as the absorber. Considering that the reduction of the thickness of cadmium telluride leads to an increase in its deficiency, and on the other hand, according to Figure 4, the variations in the efficiency is less for the thicknesses less than 0.7 µm, this ratio of thickness has been considered for the absorber layer. Afterward, for this thickness ratio of the absorber layers, the influence of other parameters on the cell's capability was surveyed.

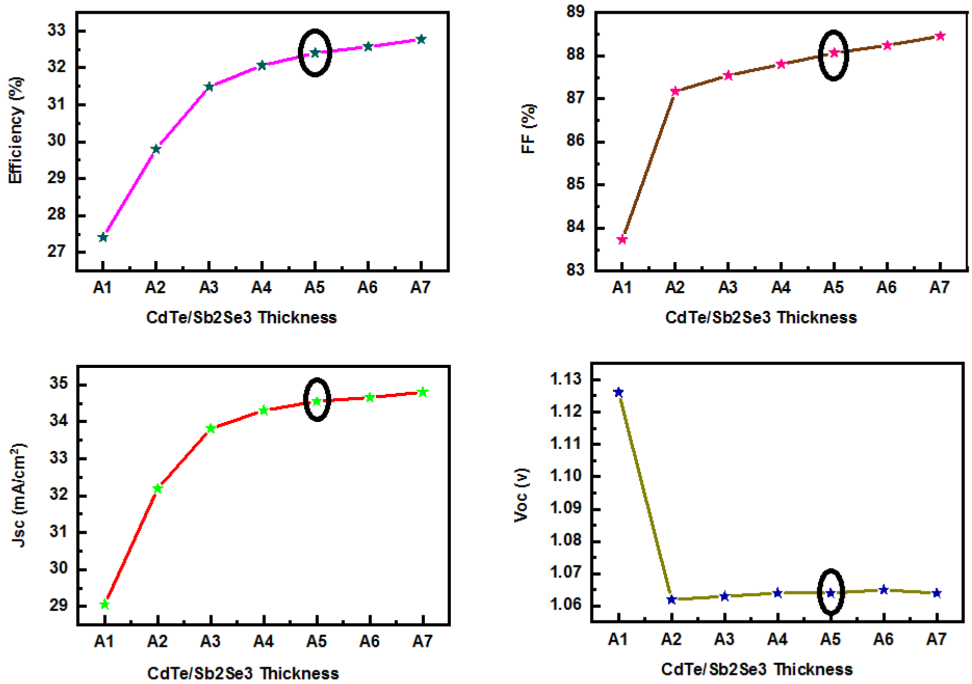

Fig. 4 Influence of absorber layers thicknesses on the characteristics of the solar cell

3.2. Effect of Band Gap Energy of Sb_2Se_3 Layer

Depending on the deposition methods, Sb_2Se_3 has a direct band gap among 1-1.5 and 1.2-1.9 electron volts. Figure (5) shows the effect of band gap energy in this range. As the band gap energy of Sb_2Se_3 increased, the short-circuit current decreased, as a result of the decrease in photon absorption at longer wavelengths $E_g > E_{ph}$. The V_{oc} is also first enlarged and then fixed. By change in bandgap, the variation in V_{OC} is in inverse direction of I_{SC}. The V_{OC} increases with bandgap. But for bandgaps larger than 0.4 eV, due to the increase in recombination, its increase is stopped and approximately is fixed. As the energy gap increases, FF and output efficiency firstly increase and then decrease. Maximum efficiency is achieved in E_g=1.33ev (32.40%). In fact, the combined effects have led to an increase in P_m in E_g=1.33 ev, where the increase in V_{oc} has covered the decrease in J_{SC} .

3.3. The Effect of Sb_2Se_3 Impurity Concentration (N_A)

N_A plays an important role on cell efficiency. In Figure 6, N_A changes in the range of 10^{13}-10^{18} cm^{-3}. It can be seen that the increase of N_A has led to the improvement of FF and thus the efficiency. The higher efficiency is obtained at higher Sb_2Se_3 concentration. Minority carriers life time is proportional to the added impurity. The higher N_A, the longer life time, which means collecting more photons at absorber layer and increase in efficiency and FF.

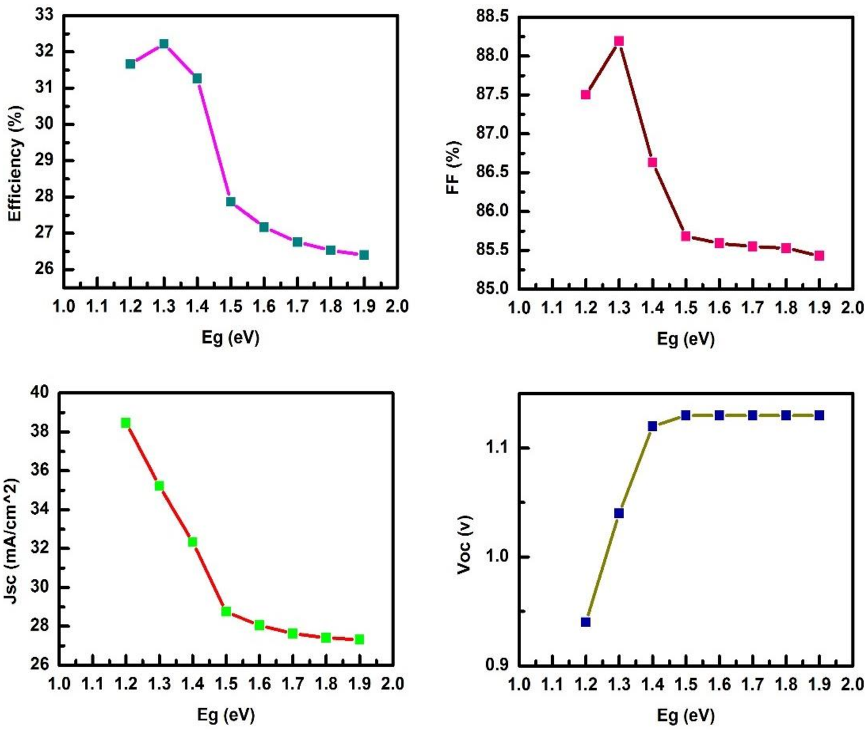

Fig. 5 The influence of band gap energy on V_{oc}, J_{SC}, FF and η

3.4. The Temperature Effects

The temperature affects the band gap of semiconductors. The band gap energy of a semiconductor decreases with growing the temperature. For temperatures more than 300K, the band gap changes can be studied according to the following equation:

$$E_g(T) = E_g(0) - \alpha \frac{T^2}{T + \beta} \tag{3}$$

in which temperature is T, $E_g(T)$ is the semiconductor band gap, and $E_g(0)$ is its value in T=0K, α and β are the connection parameters [18]. Figure 7 shows influence of increasing temperature on cell performance which are the direct results of reduced bandgap energy by temperature. Due to the importance of temperature effects on cell performance, its dependency is investigated in Figure 7. By increase in temperature, the velocity of carriers increases. It means higher recombination rate and reduced efficiency.

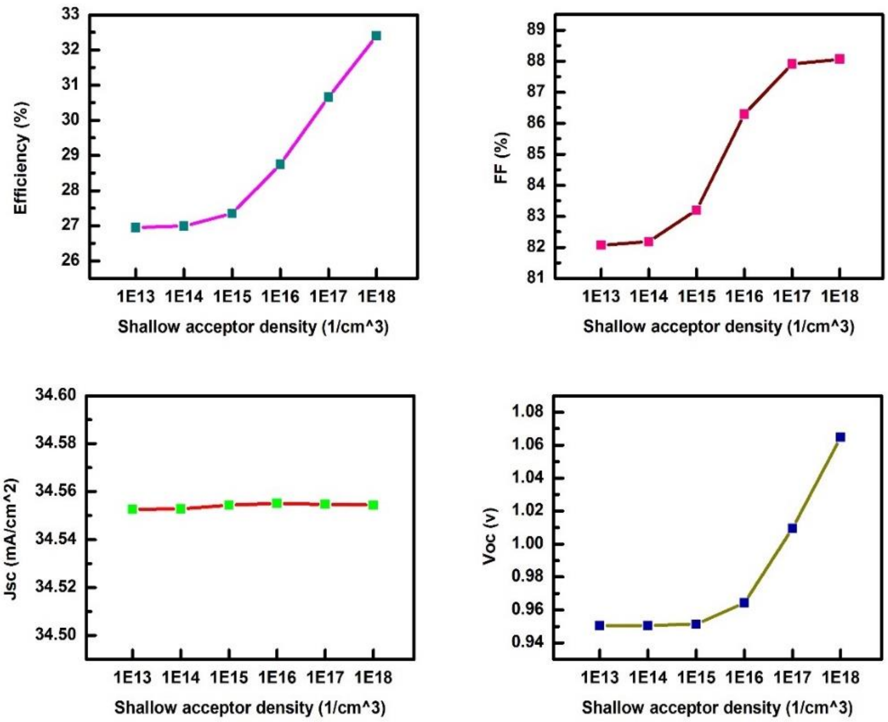

Fig. 6 Sb_2Se_3 impurity concentration effects on output parameters of the cell

3.5. Effect of Metal Work Function of Back Contact

Choosing the proper metal is essential to achieve maximum efficiency. Figure 8 shows the effect of the work function of the metal on the output characteristics of the structure. In this study, different materials such as Pt, Au, Ni, Mo, Ag, Zn, Cu, and Al have been used. As can be seen, with the growth in the metal work function, the efficiency rises, which indicates the decrease in the height of the barrier with the growth in the work function of the metal. The efficiency for work function more than 5.65ev is fixed.

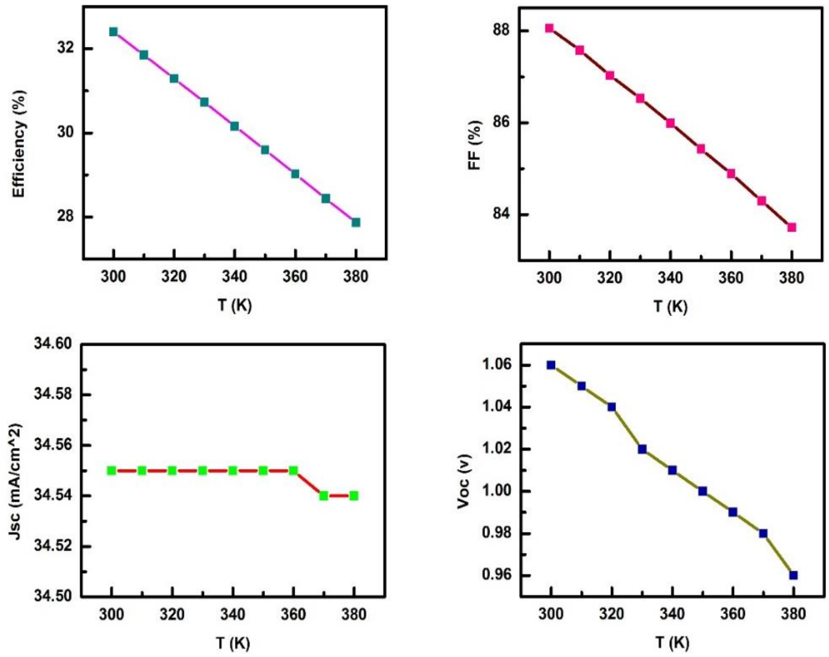

Fig. 7 Characteristics of the Sb_2Se_3/CdTe solar cell versus the operating temperature

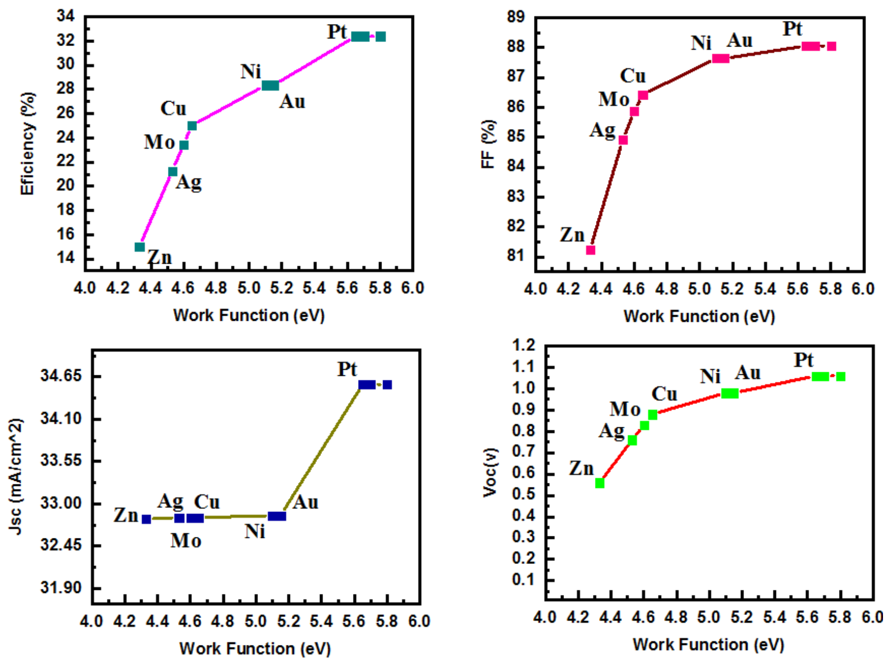

Fig. 8 Result of metal work function change on V_{oc}, FF, J_{SC}, and η

3.6. Energy Band Diagram, QE and Current-Voltage Curve

Figure 9a illustrates energy band diagram of SnO_2:F/ZnO/CdS/CdTe/Sb_2Se_3/Pt structure, and 9b and 9c show QE and (J-V) curves for different band gap energy values of Sb_2Se_3 in this cell. The performance characteristics are compared with the experimentally and numerically characteristics in the other works for the CdTe based solar cells as presented in Table 4. Based on Table 4, compared to other structures, the proposed structure includes less use of a limited source material (Te). Also, its V_{OC}, I_{SC}, FF, and efficiency show that by using two absorber layers, an efficient and more compatible with environment solar cell can be achieved.

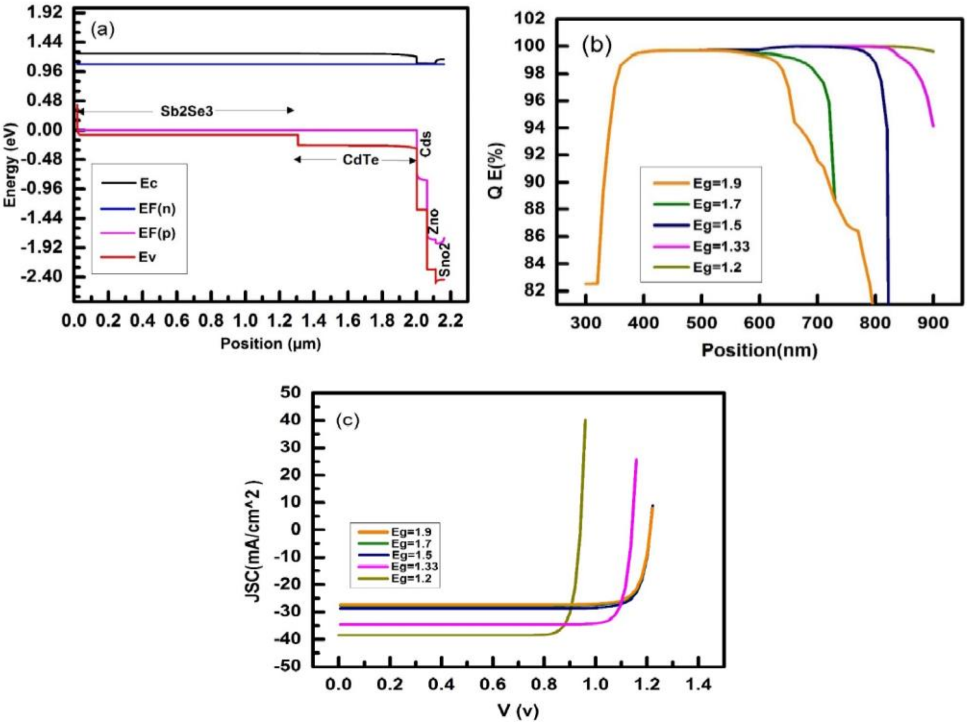

Fig. 9 (a) Energy band diagram of SnO_2:F/ZnO/CdS/CdTe/Sb_2Se_3/Pt structure. (b) and (c) QE and J-V curves for different band gap energy values of Sb_2Se_3

Table 4 Device characteristics of the proposed structure in comparison with the reported Cd cells.

Structure	Experime-ntal/ Sim ulation	Thickness of Absorber layer (μm)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	η (%)	Ref.
FTO/Cds/CdTe/BCS/ITO	Exp	3	0.823	21.2	70.4	12.3	[19]
Sno2:F/Cds//CdTe/Cd1-xMgxTe/Cu/Te /Au	Exp	3	1.01446	24.32	75.96	17.53	[13]
Sno2:F/MZO/Cds:o/CdTe/Mo/Al/Cr	Exp	3-5	0.8625	26.8	78.2	18.05	[20]
Sno2 /CdSe/CdTe/Al	Sim	4	0.870	24.32	76.19	16.13	[21]
Au/ZnTe:Cu/CdTe/Cd1-xZnxS/ITO	Sim	2.5	1.1	27.18	66.65	19.93	[22]
ZnTe/Zns/CdTe/Si	Sim	2.5	1.01	29.32	72.06	21.38	[23]
ITO/Tio2/Cds/CdTe/Mos2/Au	Sim	3	1.141	27.69	83.80	26.49	[24]
Tio2/Cds/CdTe/Cuo/Pt	Sim	3	1.107	28.48	89.10	28.11	[25]
CdTe/CISSE/Si/CdS/Zno	Sim	3	0.8136	41.1436	79.36	27.38	[26]
CuSCN/CdTe/CdS/ZnO:Al	Sim	4	1.03	27.4	80.17	22.62	[27]
FTO/MZO/CdTe/Te:Cu	Sim	2.5	0.92	26.15	87.03	21.04	[28]
SnO2:F/ZnO/CdS/CdTe/ Sb2Se3/Pt	Sim	2	1.06	34.55	86.06	32.40	This work

4. Conclusion

In this work, a solar cell based on CdTe has been designed and simulated. Firstly, the absorber layer thickness has been decreased, which led to a decrease in the cell efficiency. This drop in performance was compensated by applying the second absorber layer and designing a solar cell composed of two absorber layers. The performance of the cell with two absorber layers had a significant improvement compared to the structure composed of one layer with the same thickness. The effect of thickness ratio, energy gap, impurity density, operating function of the back contact metal, and the operating temperature on the output parameters of the structure have been investigated. The simulation outputs confirmed a higher efficient and more environmentally compatible solar cell using two absorber layers. The efficiency of 32.40% for the thickness of 1.3 μm of Sb_2Se_3 layer and 0.7 μm of CdTe layer, at the temperature of 300K was obtained. It shows 5% improvement compared to the structure with only the CdTe absorber with same absorber thickness.

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