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Rahul Raj Hazarika[1]

rahulrajhazarika0@gmail.com

Jagannath Barooah University

Pronob Jyoti Saikia

Jagannath Barooah University

Sagar Bhattari

Indian Institute of Technology Guwahati

Kangkan Bora

Jagannath Barooah University

Sawagatam deva Nath

Jagannath Barooah University

Manash Borah

Jagannath Barooah University

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Enhancing solar conversion efficiency of CdTe-based absorber solar cells via SCAPS-1D simulation

Rahul Raj Hazarika[1]*, Pronob Jyoti Saikia[2], Sagar Bhattarai[3], Kangkan Bora[1],

Sawagatam Deva Nath[1,4], Manash Bora[1],

[1]Department of Physics, Jagannath Barooah University, Jorhat, Assam, India

[2]Department of Electronics, Jagannath Barooah University, Jorhat, Assam, India

[3]Technology Innovation and Development Foundation, Indian Institute of Technology Guwahati, Guwahati, Assam, India

[4]Department of Physics, N N Saikia College, Titabor, Assam, India

Abstract:

The growing global energy demand and the need for new sources have driven significant advancements in energy storage technologies, which are essential for improving energy sustainability and efficiency. Cadmium telluride (CdTe) is one of the most efficient and cost-effective thin-film solar cell materials with an ideal band gap between 1.44 eV and 1.5 eV. CdTe is a long-standing material in the fabrication of solar cells for its ideal band gap and high optical absorption coefficient. This is a promising material due to its efficient devices and cost ratio because of its large flexibility in the manufacturing process. Due to its properties, CdTe has been regarded as a material for producing high-efficiency solar cells. In the ideal band gap range, which is suitable for the solar cell spectrum and maximum absorption (more than 90%) of incoming photons at a thickness of 2 µm. CdTe is the absorber; the cadmium sulphide (CdS) film and the back contact are the typical layers that make up the conventional structure of a superstrate CdTe solar cell. An absorber layer with Nickel oxide (NiO) as the window layer was investigated in order to enhance the Photovoltaic (PV) system's device features as well as parameters. To assess the effectiveness of the thin-film solar cell architectures, can be modelled utilising computer simulations. The efficiency of CdTe Photovoltaic (PV) cells was found to be 27.7 % by simulation in SCAPS-1D simulation software.

Keywords: Solar cells, CdTe layer, band gap, PV performance, SCAPS-1D

(*Corresponding Author: Rahul Raj Hazarika

Email ID: rahulrajhazarika0@gmail.com)

Introduction:

There are several polycrystalline semiconductor materials that can be used for solar photovoltaic applications. One of these materials has come to the forefront of solar PV technologies: CdTe. Group II–VI semiconductors, especially cadmium-based chalcogenides,

have attracted considerable research interest because of their useful electrical and optoelectronic properties. Cadmium sulphide (CdS) and cadmium telluride (CdTe) are important II–VI semiconductor materials used in optoelectronic devices and solar cells [1]. CdTe is widely studied as an absorber material in thin-film solar cells, while CdS is commonly used as a buffer or window layer in CdTe-based heterojunction solar cells. CdS thin films also have suitable optical and electrical properties, making them useful for photovoltaic and other optoelectronic applications [2]. This material is a direct band gap semiconductor (fabricated as a P-type semiconductor) and, therefore, requires only a thin layer to realise a solar cell. The band gap of CdTe is about 1.44 eV, close to the ideal band gap required. Both of these materials are deposited in the form of polycrystalline films with a grain size of the order of a few micrometres at best. But the electrical activity at the grain boundary is lower, meaning recombination at grain boundaries is not significant (in contrast to polycrystalline Si). This makes it possible to fabricate a P–N junction solar cell [3]. Due to the material's high light absorption, photons are absorbed very close to the surface, where recombination losses can be significant. In order to avoid front surface recombination, a window layer or buffer layer with a high band gap is used in both cases. CdS with a band gap of about 2.42 eV is used as a buffer layer. The N-type CdS also serves as a layer that forms a heterojunction, required for charge separation. Thus, the CdTe P-N junction solar cells are actually CdS-CdTe solar cells. Both of these cells use a transparent conducting oxide (TCO) layer to make front metallic contact. A concern of these two technologies is the use of Cd, which is a toxic material. Also, some of the materials used, like indium (In) and tellurium (Te), are not available in large quantities in the Earth's crust. Therefore, in future, material availability could be an issue. For instance, the weight percentage of tellurium (Te) in the Earth's crust is only 0.0000002 [3,4]. The weight percentage of several elements that are used in solar PV applications. Fabrication of solar cells based on thin, crystalline silicon films appears to be one of the most attractive routes to produce cheap and efficient solar cells. Crystalline silicon is an excellent material for solar cells, and its use in thin-film technology will also continue for many reasons. It has proven to provide high and stable cell efficiencies. It is non-toxic, and the raw material is abundantly available in nature, which is a significant advantage compared to thin-film compound solar cells such as CdTe [4-6].

CdTe has an important advantage because it can show both p-type and n-type conductivity. Although CdTe has been studied for many years, its use in quantum dots and polycrystalline thin films for solar cells has grown more recently. Studies show that CdTe can provide good efficiency and stability, making it a promising p-type absorber material for thin-film solar cells. The growing demand for low-cost and environmentally friendly energy has increased interest in photovoltaic (PV) technology [7]. Thin-film solar cells use very small amounts of semiconductor material, which can help reduce the overall cost. Researchers are also working to develop solar cells that are lightweight, flexible, efficient, affordable, and less harmful to the environment. Therefore, CdTe is being studied as a suitable absorber material for thin-film solar cells, with the goals of reducing cost, improving efficiency, and reducing the use of

harmful materials. SCAPS software is widely used to design, simulate, and analyse the performance of solar cells before fabrication [7-9].

Materials and methods:

In this paper, we proposed a solar cell with the model *"Back Contact/ NiO /CdTe/ CdS /Front Contact"*. This solar cell has a structure consisting of CdS, NiO, CdTe, as well as Au layers. To study the effectiveness of CdTe as an absorber in photovoltaic cells. The device structure is developed using SCAPS-1D simulation (version 3.3.7). In device CdTe takes as absorber CdS as electron transport layer (ETL) and NiO is hole transport layer (HTL) for the window absorber in proposed cell model. These materials have sustainability as well as effectiveness. The device efficiency is improved by varying layer thickness, doping concentration, and defect density, and we calculate short-circuit current density, fill factor, open-circuit voltage, and power conversion efficiency in the simulation [4-7]. In Table:1 [3,7,8], the material properties: bandgap energy, mobility, electron affinity, and doping concentrations are chosen, and they are presented. From a research perspective, we aim for CdTe solar cells to achieve high efficiency and good stability, but some important problems still need to be solved. One major problem is the use of tellurium (Te), which is a rare and costly material. The limited availability of Te can make it difficult to produce CdTe solar cells on a large scale. Although CdTe is a good material for absorbing sunlight, more research is needed to reduce the amount of Te used without reducing the efficiency and performance of the solar cell. This is especially important for developing ultrathin CdTe solar cells that use less material and are more sustainable [10-14].

For modelling, we are using the Solar Cell Capacitance Simulator in 1 Dimension (SCAPS-1D) *(version 3.3.07; URL: https://scaps.elis.ugent.be/)* to analyse how the thicknesses of the electron-transport layer (ETL) and the absorber layer, as well as defect densities, affect device performance [11,12]. The structure of the simulated solar cell is shown in Figure 1.

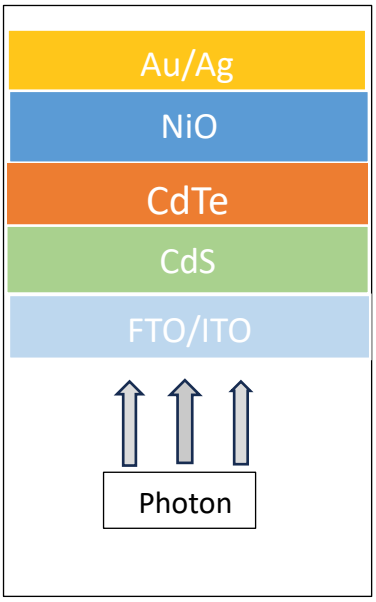


Figure 1. Solar cell model in Simulation

Table 1: Parameters of the materials in the perovskite solar cell

Parameter (unit)	**NiO**	**CdTe**	**CdS**
Layer Thickness (µm)	0.050	2.000	0.100
Eg (eV)	3.800	1.440	2.420
E affinity (eV)	1.450	4.280	4.400
Dielectric permittivity(relative)	10.700	10.300	10.000
CB DOS (cm−3)	2.800E+19	1.000E+17	1.200E+18
VB DOS (cm−3)	1.000E+18	1.000E+18	1.800E+19
Electron thermal Velocity (E)(cm/s)	1.000E+7	1.000E+7	1.000E+7
Hole thermal Velocity (H)(cm/s)	1.000E+7	1.000E+7	1.000E+7
Electron mobility (cm2/V s)	1.200E+7	1.000E+2	1.000E+2
Hole mobility (cm2/V s)	2.800E+0	1.000E+1	5.000E+1
N_D (cm−3)	-	-	-
N_A(cm−3)	0	0	0
Defect type	1.000E+19	2.000E+20	2.100E+17

CdTe absorber conventional model:

In this PV solar cell, CdTe is taken as a single absorber layer. The CdTe absorber layer shows good performance up to a thickness of 2 µm, beyond which the improvement becomes insignificant. Increasing the absorber-layer thickness enhances light absorption, particularly in the infrared region. Therefore, the overall performance of the solar cell is strongly influenced by the thickness of the absorber layer. In the experimental process, the manufacturing of CdTe materials is achievable on Earth. Increasing the thickness of the CdTe absorber layer enhances the power conversion efficiency (η) by increasing the amount of solar energy absorbed. At a thickness of 2 µm, correspondingly, the effectiveness (η) is more than 24% [15]. Furthermore, changes in the absorber-layer thickness result in corresponding variations in the open-circuit voltage (V_{0c}) and short-circuit current density (J_{sc}) of the PV cell. To analyse the performance of the solar cell, a one-dimensional software, SCAPS-1D, is used. The solar cell model consists of a CdS buffer layer, a CdTe absorber layer, and a NiO window layer. Appropriate boundary conditions are applied to represent the behaviour of the electrodes. Both the front and back contacts are assumed to be ideal ohmic contacts to ensure efficient charge-carrier collection. The increasing global demand for energy has created a need for clean and renewable energy sources. Among various photovoltaic technologies, CdTe solar cells have attracted considerable attention because of their high efficiency, low cost, and relatively simple fabrication process. However, conventional CdTe solar cells usually require a thick CdTe layer, which increases material use and production cost. Therefore, researchers are developing CdTe

solar cells that use less material while maintaining good performance. Single- and double-absorber-layer structures can help improve light absorption and the collection of charge carriers [16-18]. Reducing the thickness of the CdTe absorber layer to an ultrathin scale can reduce charge-carrier recombination and enhance charge-carrier transport. These lightweight and flexible solar cells may be useful for mobile devices, wearable technology, and building-integrated solar systems. However, challenges such as absorbing enough sunlight with a thin layer and maintaining long-term stability still need to be solved. Thus, research on ultrathin CdTe solar cells is important for developing low-cost, lightweight, efficient, and environmentally friendly solar energy technologies. Solar cell characteristics utilised in our simulation were chosen from academic literature, theories, and experiment-based results as shown in Table 1. The lighting spectrum is adjusted, and the temperature is set to 300K [19,20]. Computer-based simulation software allows time and money to be saved. It predicts and evaluates the effects of various model parameters and material properties on the performance of the solar cell. In this work, we use SCAPS-1D software developed by Marc Bargeman and colleagues at the University of Gent [13,14].

Numerical Analysis:

When modelling solar cells, ensure that the program can solve Poisson's equation for the electrostatic charge potential $div(\varepsilon \nabla \Psi) = -\rho$ [11], as well as the carrier continuity equations for electrons and holes (i) and (ii) [12].

$$\frac{\partial^2 n}{\partial t} = \frac{1}{q} div \overrightarrow{J_n} + G_n - R_n \qquad \text{(i)}$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} \mathrm{div} \overrightarrow{J_p} + G_p - R_p \qquad \text{(ii)}$$

Where,

n=$concentration\ of\ electrons$, p = $concentration\ of\ holes$, J_n=$Electron\ current\ density$, J_p=$Hole\ current\ density$, G_n= $Electron\ Generation\ Rate$, G_p= $Hole\ Generation\ Rate$, R_n= $Electron\ Recombination\ Rate$, R_p= $Hole\ Recombination\ Rat$e.

The effect of CdTe thickness and absorption coefficient variation has been examined as well as effect of different temperatures on the performance of solar cell was then simulated [24]. The solar cell parameters used in the simulation are listed in Table 1. Whereas, parameters for both front and back contacts are shown in Table 2.

Table 2: Simulation Parameters used for back and front contacts from SCAPS-1D [23-25].

Parameters	**Front contact**	**Back contact**
Surface recombination velocity of electrons (cm/s)	1.00×10^7	1.00×10^5
Surface recombination velocity of holes (cm/s)	1.00×10^5	1.00×10^7
Metal work function (eV)	4.6239	5.7973
Majority carrier barrier height relative to Ef (eV)	0.053	0.152
Majority carrier barrier height relative to Ev (eV)	0.0000	0.0000

Results and discussion:

CdTe absorber layer thickness was systematically identified in the simulation to achieve an optimal balance between carrier collection, photon absorption and recombination losses. As expected, increasing the CdTe thickness initially improved short-circuit current density (J_{sc}) and power conversion efficiency (PCE) due to enhanced light absorption [17]. However, beyond approximately 2 µm, performance gains saturated as recombination began to offset additional photogeneration, consistent with established behaviour in thin-film solar cells. To investigate the current density-voltage (J-V), open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), Power Conversion Efficiency (PCE), as well as Fill Factor (FF). The effect on final output device factors like J_{sc}, v_{0c}, FF, PCE, and quantum efficiency (QE) were examined after the thickness was progressively changed from 0.2 µm to 2 µm. CdTe having a thickness of 2 µm may absorb 90% of the light in that particular wavelength band. The thickness of 2 µm was used to get the short-circuit current (J_{sc}) value of 27.7 mA/cm². While the CdTe layer thickness was near 2.00 µm, the Voc (open-circuit voltage) remained constant because Jsc was constant and the saturation current density was unaffected by the layer's thickness [18,19]. The absorbance coefficients related to NiO, CdS, and CdTe were systematically assessed following their synthesis by a simple chemical procedure. The experiment's absorption coefficient information was further analysed in SCAPS-1D to determine the influence of these materials on solar cell efficiency, which was found to be 27.7 %. As Figure 2 shows, the characteristics of current density-voltage (J-V).

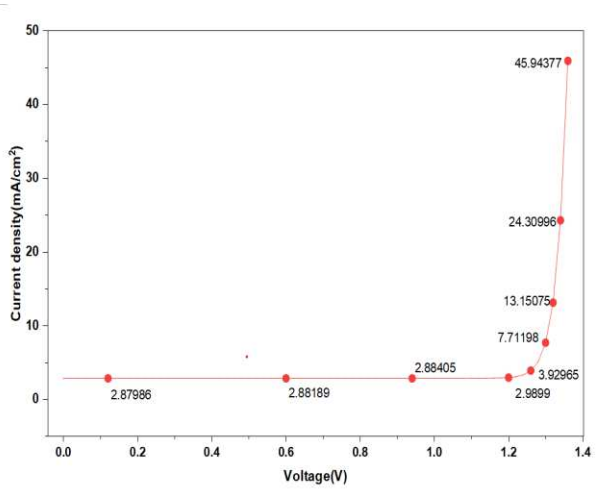


Figure 2: Current density-voltage (J-V) of absorber CdTe

Adjusting the bandgap and energy levels of materials in a perovskite solar cell (PSC) is important for improving charge transport and overall device performance. For electrons to move easily from the absorber layer to the electron transport layer (ETL), the conduction band (CB) of the absorber should be slightly higher than the CB of the ETL [8]. Similarly, for holes to move efficiently, the valence band (VB) of the hole transport layer (HTL) should be slightly lower than the VB of the absorber. This proper energy-level alignment helps electrons and holes move smoothly through the solar cell [16].

Figures 3, 4 and 5 show how interface thickness and total defect density affect the performance of CdTe solar cells with absorber layers. When the interface defect density increases, more electrons and holes recombine. As a result, the efficiency, open-circuit voltage (Voc), fill factor (FF), and short-circuit current density (J_{sc}) decrease. Therefore, reducing interface defects is important for improving the performance of CdTe solar cells. The density-voltage characteristics related to ultrathin CdTe PV solar cells with a single (CdTe) layer are shown in this image [14,16,23]. The absorber provides a better power conversion efficiency (27.7%) owing to its enhanced short-circuit current density v_{oc} and FF. Better current density as well as voltage characteristics demonstrate the absorber's enhanced functionality as well as its potential to increase device effectiveness [24].

(i) Contour plot of Thickness Vs Thickness of Absorber (CdTe)

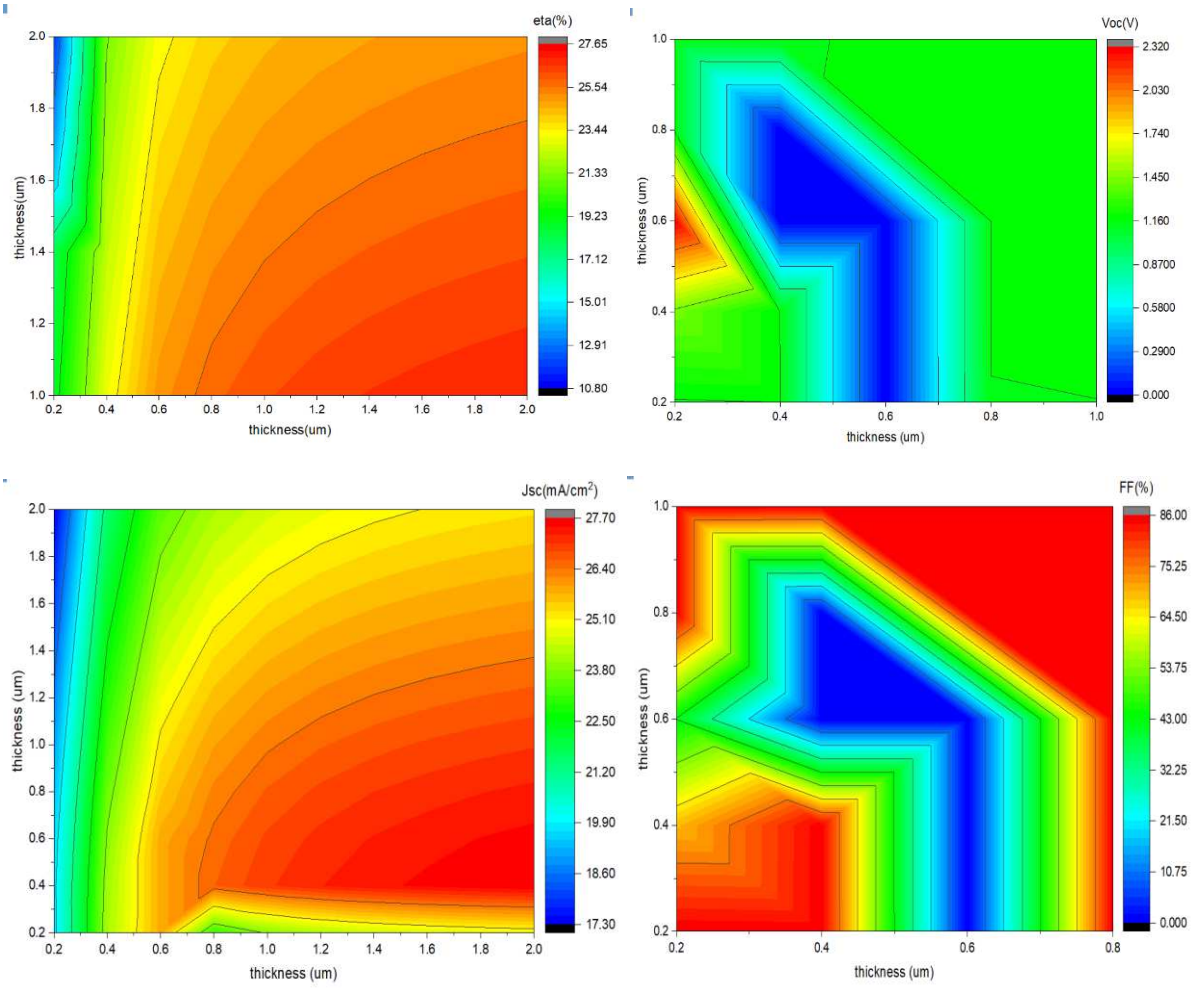


Figure 3: Variation in PV parameters of PSC [**eta,** v_{oc}**,** J_{sc} and **FF**], influenced by the thickness vs. thickness of the CdTe absorber layer.

(ii) Contour plot of thickness vs. total defect density of absorber (CdTe)

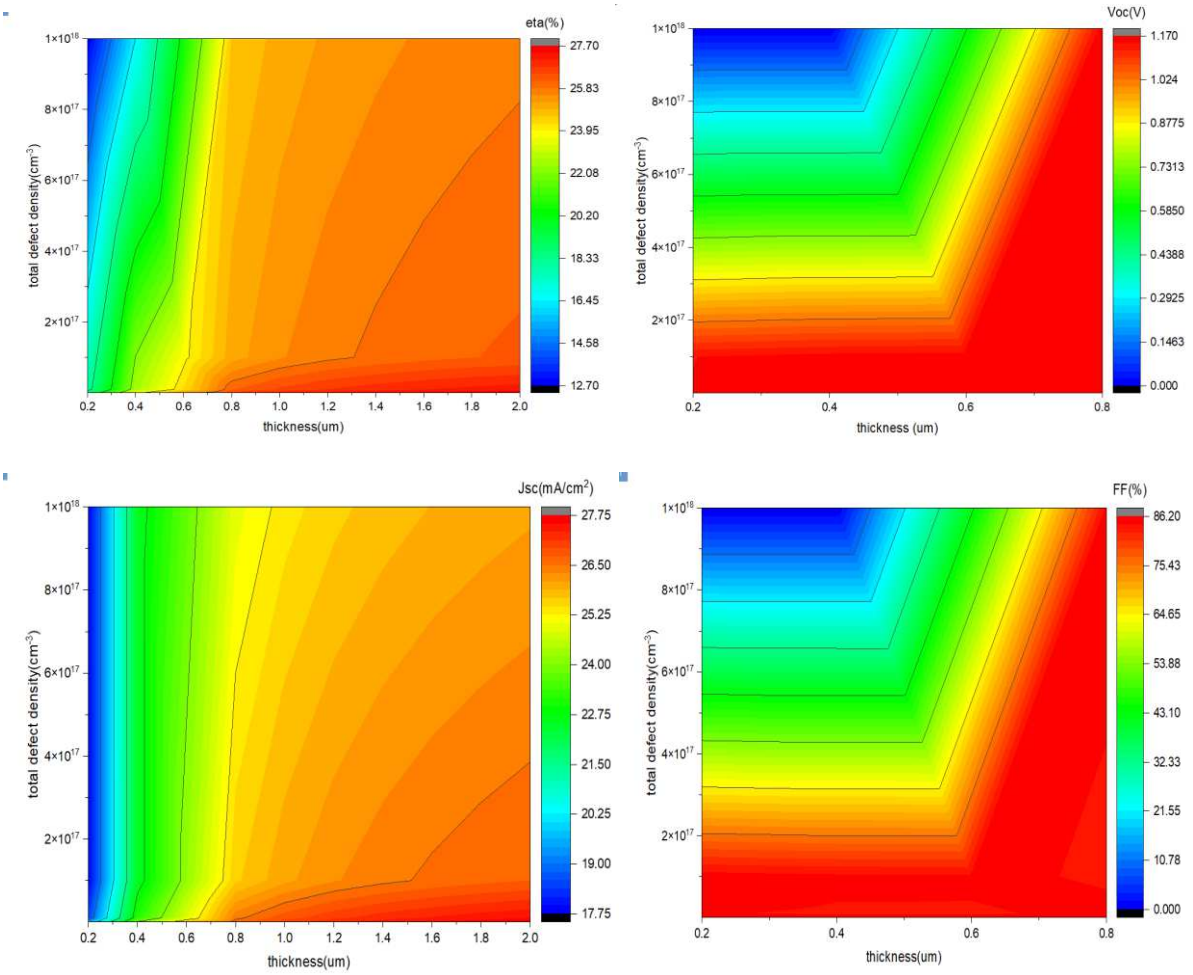
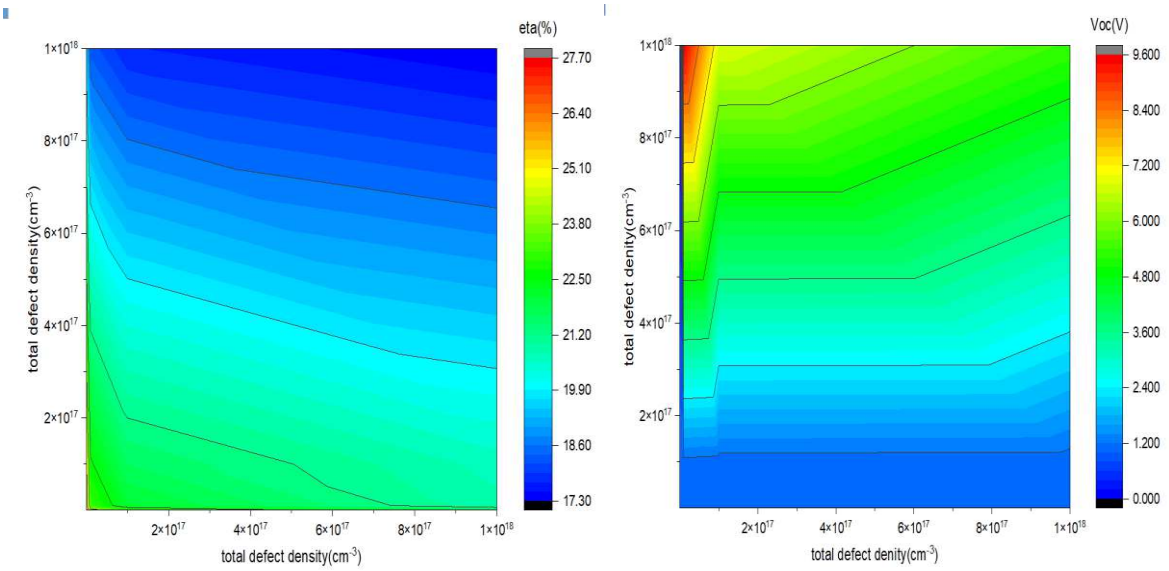


Figure 4: Variation in PV parameters of PSC [**eta,** v_{oc}, J_{sc} and **FF**], influenced by the thickness vs. total defect density of the CdTe absorber layer.

(iii)Contour plot of Total defect density vs. total defect density of absorber (CdTe)



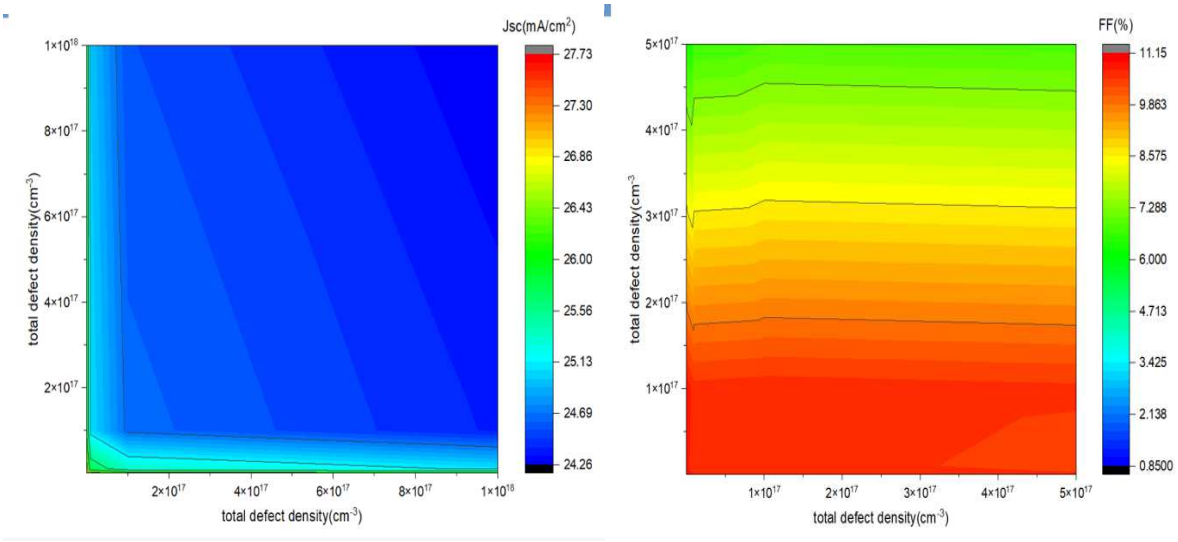


Figure 5: Variation in PV parameters of PSC [**eta,** $\boldsymbol{v_{0c}}$**,** $\boldsymbol{J_{sc}}$ and **FF**], influenced by the thickness vs. total defect density of the CdTe absorber layer.

Impact of CdTe absorber layer thickness:

The thickness of the absorber layer is an important factor that affects solar-cell performance. In this study, the thickness of the CdTe absorber layer is varied from 0.2 µm to 2 µm to study its effect on J_{sc}, FF, $v_{oc}$and efficiency. As the CdTe thickness increases, the short-circuit current (J_{sc}) and fill factor (FF) increase slightly. The open-circuit voltage (v_{Oc}) depends on factors such as light intensity, temperature, carrier mobility, and bandgap. The open-circuit voltage (v_{0c}) also increases slightly with increasing CdTe thickness, mainly due to improved hole mobility. Therefore, the relationship between Voc and J_{sc} can be expressed using the following equation [20].

$$v_{oc} = \frac{nkT}{q} \cdot ln\left(\frac{Jsc}{J_0} + 1\right) \qquad \text{(iii)}$$

Where k represents the Boltzmann constant, and T is the temperature. As illustrated in Figure 6, J_{SC} increases as the thickness rises because the active layer absorbs more photons. The decrease in current density results due to the less production of electron–hole pair as less number of electron–hole pair can reach the absorber layer. Equation (iii) states that a lower value is J_0 necessary for a higher v_{oc} [20,21].

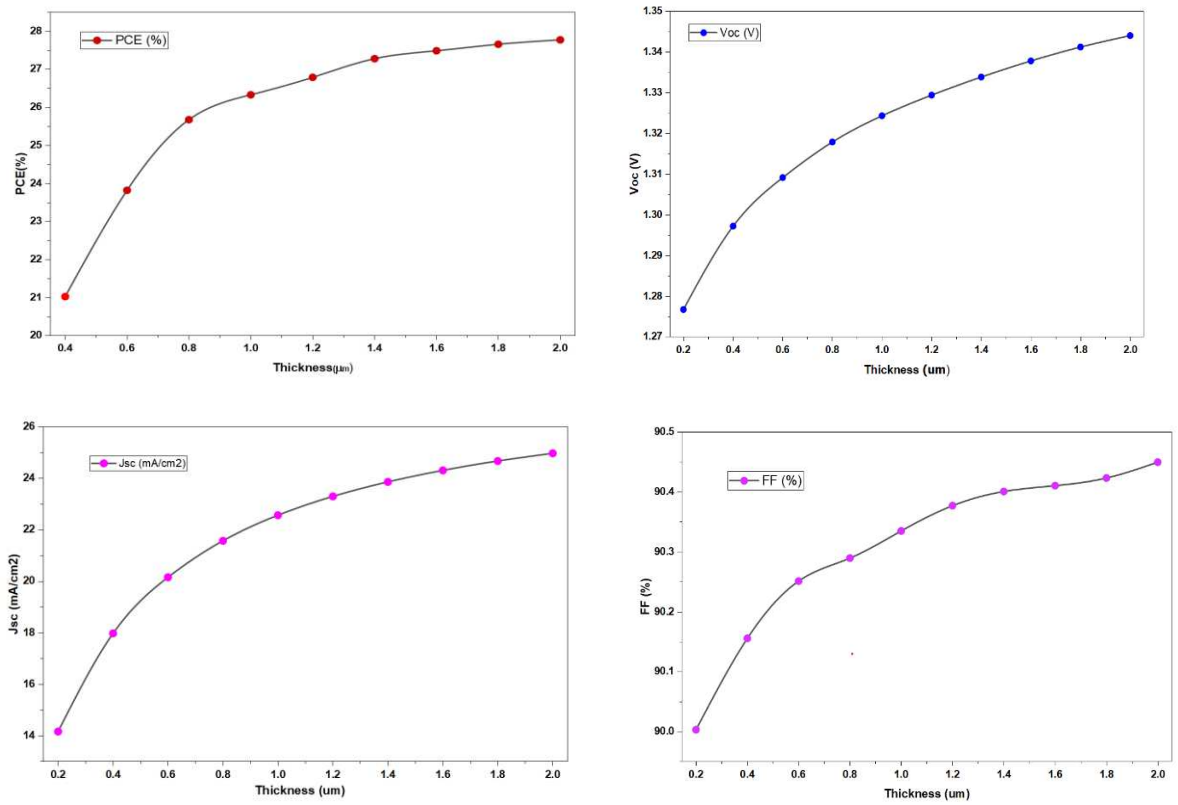


Figure 6: The influence of thickness on [**PCE,** v_{oc}**,** J_{sc} and **FF**] of CdTe.

Impact of the HTL thickness and Defect density on outputs.

After determining the optimum absorber thickness, the effect of NiO as the hole transport layer (HTL) is studied to improve hole extraction and reduce recombination losses. Figure 7 presents the dependence of eta, v_{OC}, J_{sc} and FF on the thickness of NiO and the defect density of the HTL. The HTL thickness varied between 0.010 and 0.050 µm, while the defect density ranged from 10^{13} to 10^{18} cm^{-3}. As can be seen from the contour plots, the higher NiO thickness leads to an increase in the efficiency of the solar cell.

Improvement in terms of thickness is noted for all four characteristics of the device. As the NiO becomes thicker, the regions related to higher values of eta, Voc, Jsc, and FF also cover a wider area, with the maximum efficiency being recorded when the thickness is about 0.050 µm. In such a case, the eta or PCE of the cell is around 27.7%, alongside the Voc value of about 1.375 V, Jsc value of 26.89 mA cm^{-2}, and FF value close to 75.22%. The improvement in terms of thickness is noted due to the fact that NiO does not serve as an absorber but acts as a hole-selective layer [15].

A different trend is observed when the defect density in the HTL increases. Although the optimum thickness remains close to 0.050 µm, the high-performance region becomes progressively smaller as the defect density rises from 10^{13} to 10^{18} cm^{-3}. The contour maps reveal that PCE is the most sensitive parameter, followed by Jsc and Voc, while the variation

in FF is comparatively moderate. This behaviour indicates that additional defect states promote non-radiative Shockley–Read–Hall recombination, allowing more carriers to recombine before reaching the contacts and thereby reducing the overall conversion efficiency [19].

The interplay between the results from the contour plots indicates that optimising the electrical characteristics of the HTL layer is as crucial as choosing its thickness. In the considered range, an increase in the NiO thickness is helpful for carrier extraction, but the effect becomes less pronounced in the case of a high defect density. Consequently, the highest device efficiency is achieved by employing a 0.050 µm NiO layer with low HTL defect density, since in this case charge transport is better and losses due to recombination become smaller. This finding is supported by recent numerical analysis, which demonstrated that transport layer optimisation is the most effective at a low defect density [16,18].

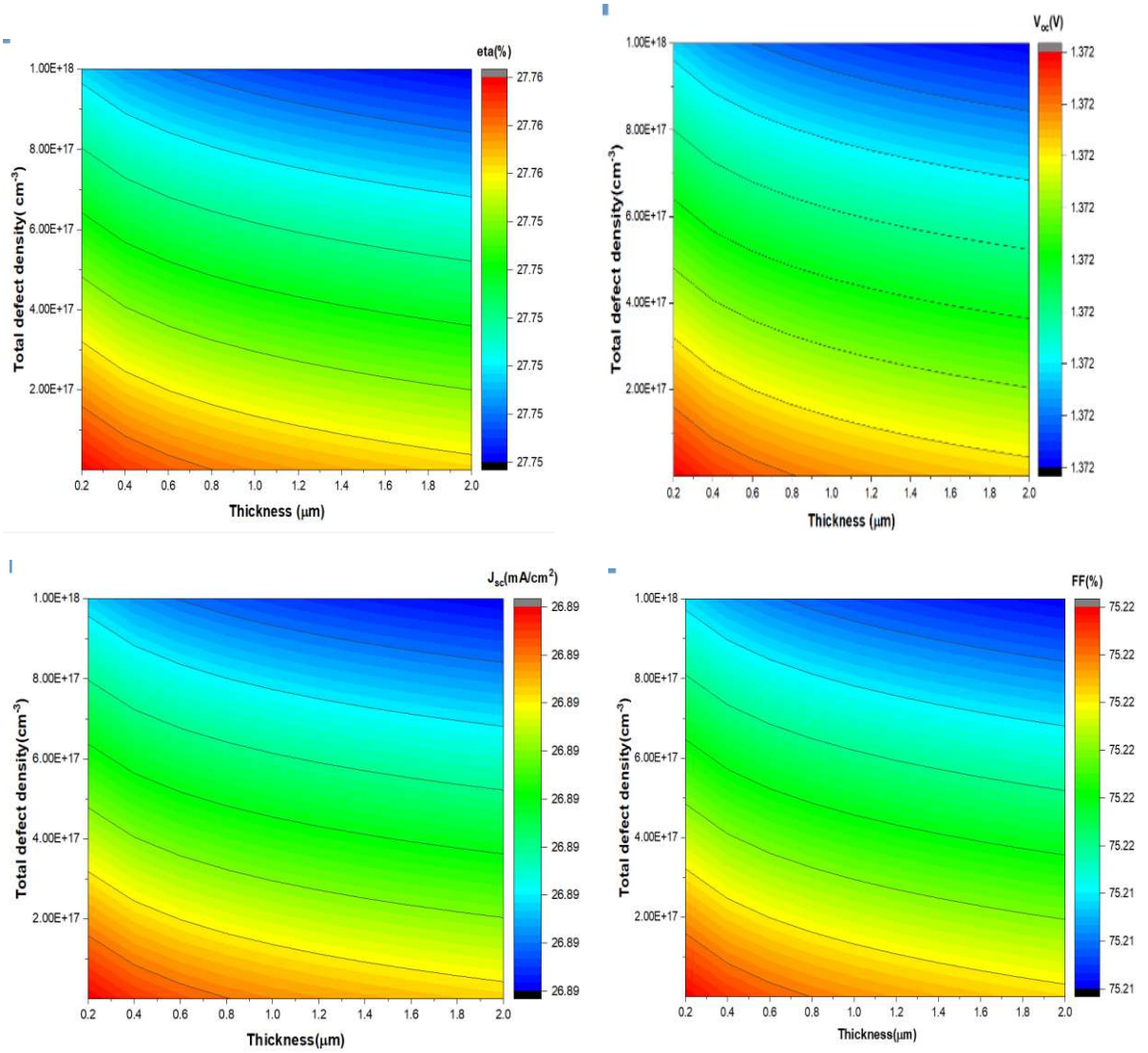


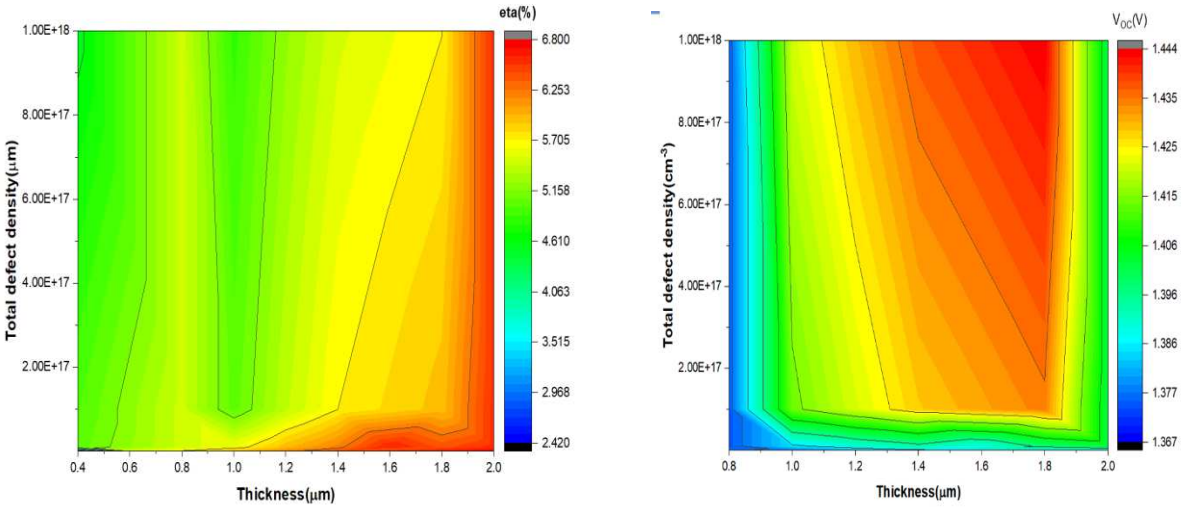
Figure 7: Presents the dependence of **eta,** v_{Oc} , J_{Sc} and **FF** on the thickness of NiO and the defect density of the HTL

Combined impact of ETL layer thicknesses and Defect density on the performance of the device

After establishing the optimum hole transport layer, the performance of the CdS electron transport layer was examined by varying both its thickness and defect density. Rather than influencing each photovoltaic parameter independently, Figure 8 shows a remarkably similar contour pattern for eta, Voc, Jsc and FF. In every case, the highest-performing region is confined to the lower-left corner of the contour maps, corresponding to a thin ETL with a low defect density. As either variable increases, this region steadily contracts, indicating that efficient electron extraction depends on the combined optimisation of both structural and electrical properties of the transport layer [9-12].

This change becomes most evident in the PCE contours. Rather than having the drop in efficiency occur immediately, the contour lines become displaced in the direction of lower efficiencies as the CdS layer thickens from 0.05 to 0.100 µm. The displacement indicates that increased thickness of the transport layer means higher resistance for electrons, which makes it less efficient for carrier collection. There is a similar trend seen in the Jsc contours, where the drop in current occurs in nearly the same direction as the displacement in efficiency contours. These trends suggest that the cause of the decrease in efficiency is charge collection efficiency, rather than optical absorption.[22]

The case is different for Voc and FF. Despite their decreasing trends with the increase in thickness and defects, contour gradients of both Voc and FF are smoother compared to those of PCE. Thus, the electrical properties of the junction remain relatively constant, whereas the process of carrier transport becomes increasingly challenging. Due to the rise in the defect density up to 10^{18} per cm^3, the contour lines become more compressed and closer to lower values due to the enhanced trapping of carriers and recombination in the ETL and the interface between the CdTe and CdS [20].



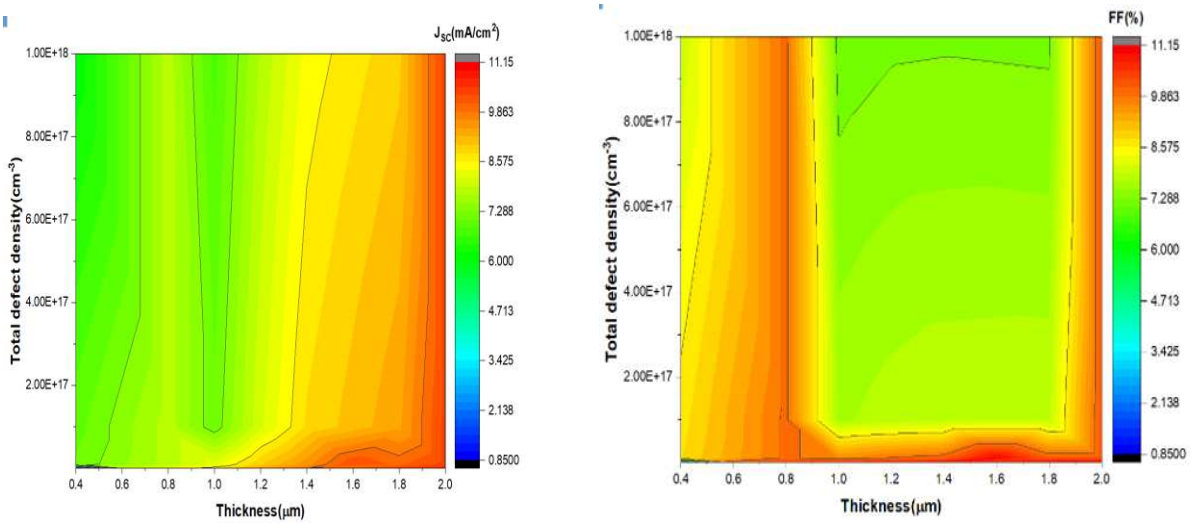


Figure 8: Presents the dependence of **eta,** v_{Oc} **,** J_{sc} and **FF** on the thickness of CdS and the defect density of the ETL

Taken together, the contour maps suggest that ETL thickness alone does not determine device performance. A thin transport layer is beneficial only when accompanied by good electrical quality, whereas increasing defect density suppresses the advantage gained from thickness optimisation. Within the studied range, a CdS thickness of 0.100 µm and a defect density of 10^{13} cm^{-3} provide the best performance, resulting in the highest power conversion efficiency PCE, Voc, Jsc, and FF. Similar conclusions have been reported in recent numerical optimisation studies of CdTe solar cells, where reducing transport-layer resistance together with interface recombination led to significant improvements in device efficiency [21].

Quantum Efficiency Analysis:

The Quantum Efficiency (QE) curve is an indication of the capability of the solar cell in converting incident photons to charge carriers at various wavelengths. This also shows how well the solar cell absorbs light and collects charge carriers [22]. The simulated device achieves a high quantum efficiency of 88–90% at wavelengths between 500 and 680 nm, indicating that it absorbs visible light effectively and collects the generated charge carriers efficiently. Past 700 nm, the Quantum Efficiency drops sharply to nearly zero at 720 nm as shown in Figure 9, which corresponds to the cut-off wavelength due to the absorption limit of the absorber layer. This is because the cut-off wavelength depends on the absorber band gap (1.44- 1.45 eV) [25].

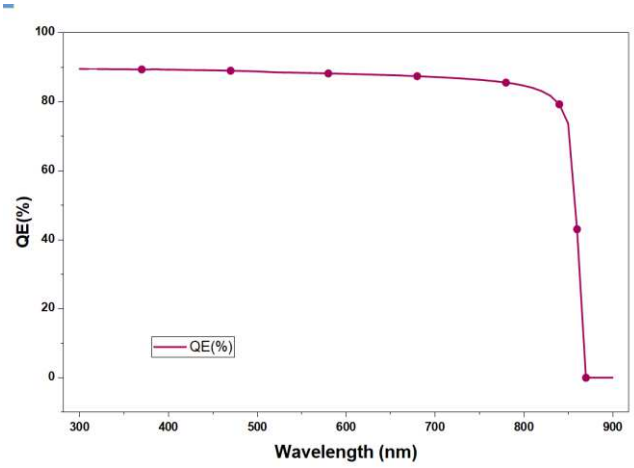


Figure 9: quantum efficiency (QE) of absorber CdTe

The performance of the solar cell as a function of temperature

Figure 10 investigates the temperature-dependent performance characteristics associated with solar cells using a single (CdTe) absorber. As temperature rises, efficiency, FF, short-circuit current density, and Voc all decrease due to increased carrier recombination as well as decreased carrier mobility. Over the whole temperature range, the absorber configuration continuously demonstrates improved thermal stability as well as efficiency preservation at higher temperatures [3,4].

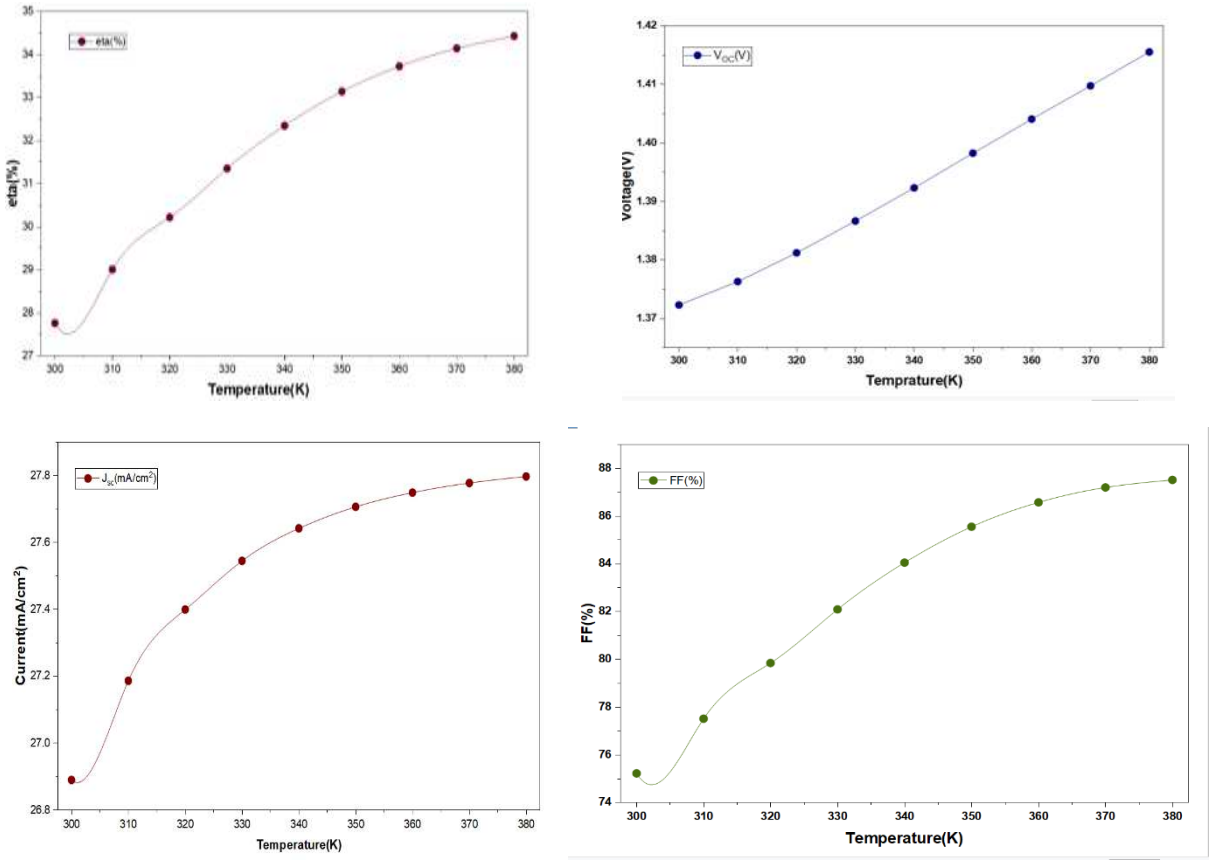


Figure 10: Photovoltaic characteristics due to temperature

Influence of resistances on PV performance

The value of series resistance as well as shunt resistance has a significant impact on the characteristics of PV cells. These considerations also dictate the features of the nodes and how they impact the performance of the device. To analyse the dependency of Rs as well as Rsh, the remaining optimised parameters from the previous section were maintained. For this simulation, the values related to Rs as well as Rsh were adjusted within the corresponding ranges of 10–100 Ω-cm². The effect of Rs as well as Rsh on the variables affecting a PV cell's effectiveness is shown in Figures 11 and 12 [13].

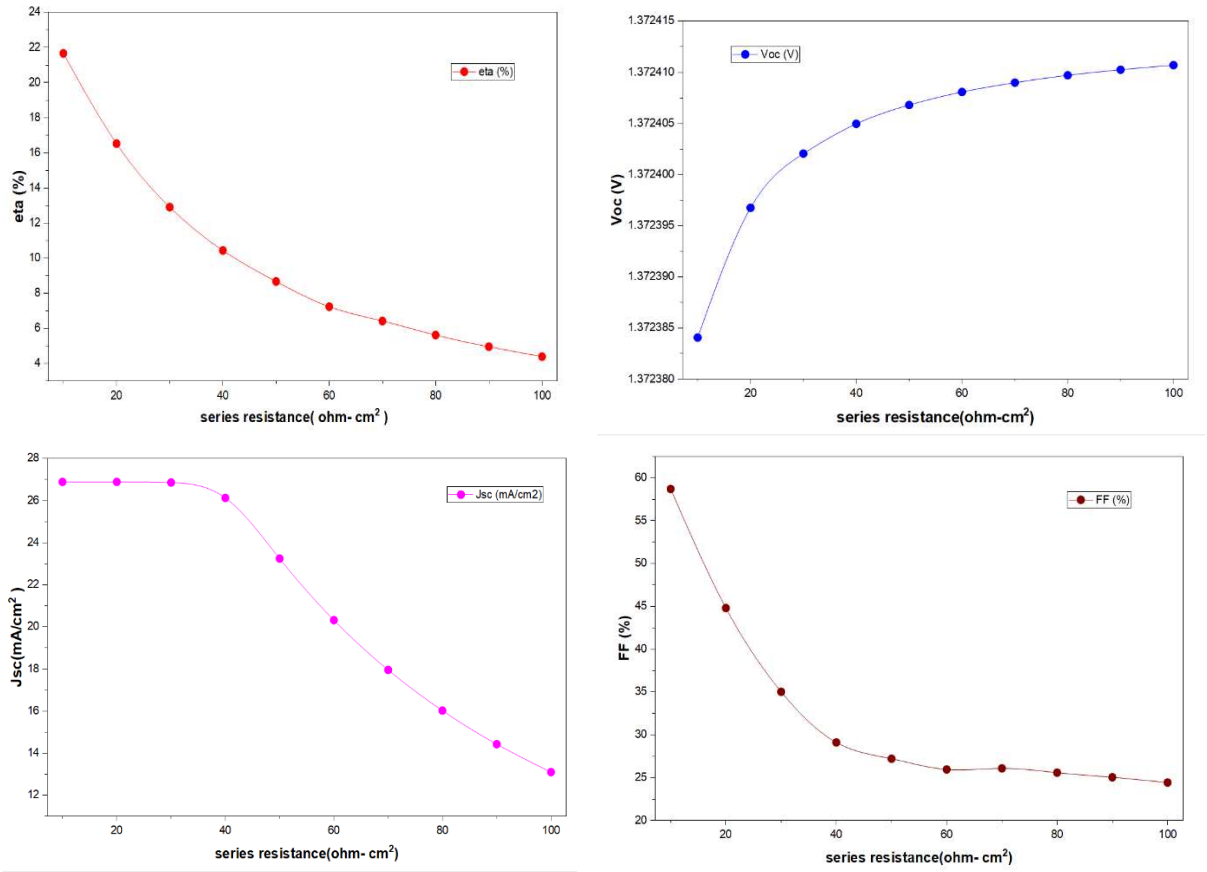


Figure 11: The influence of series resistance (Rs) with the absorber**.**

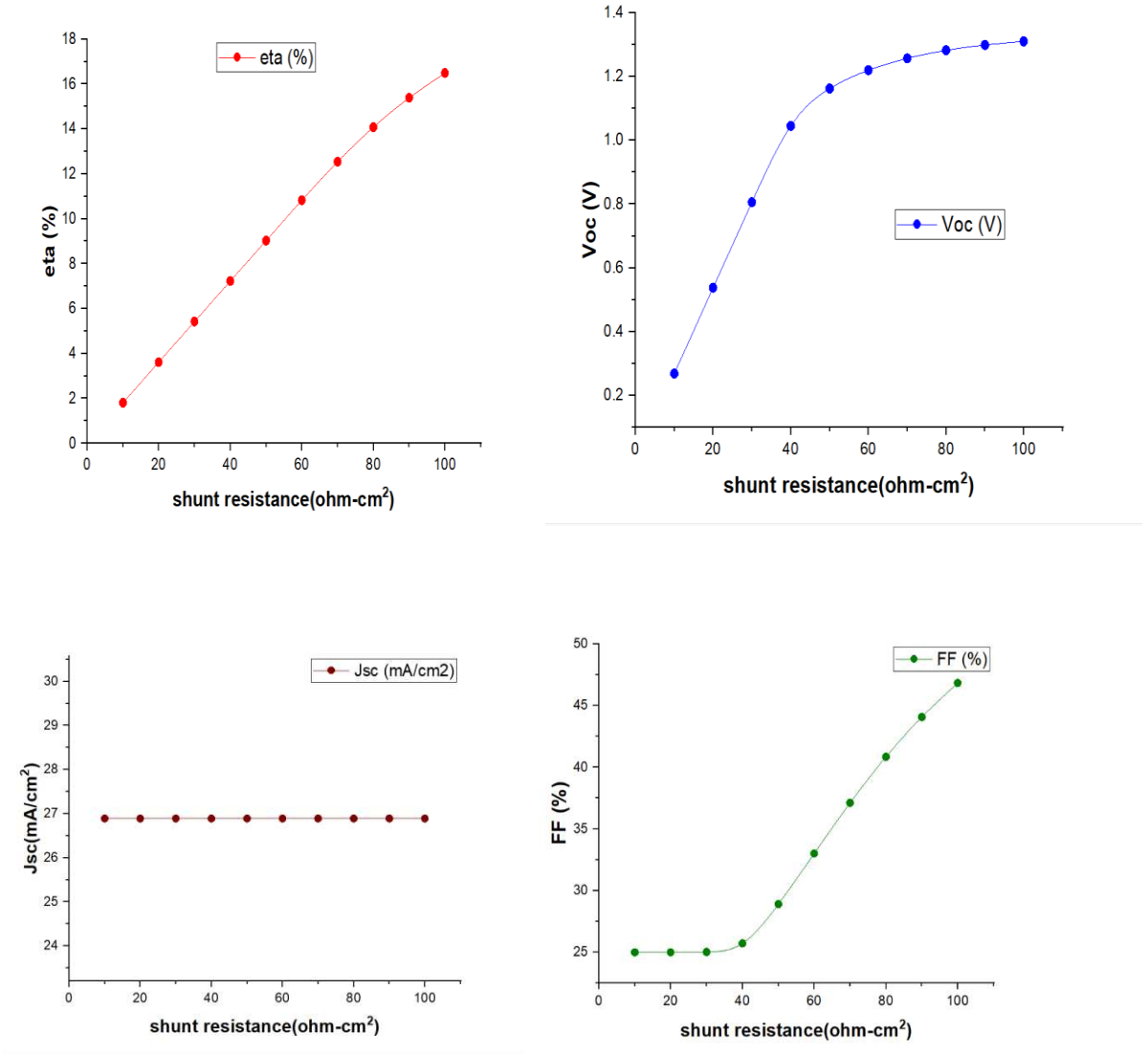


Figure 12: The influence of shunt resistance (Rsh) with absorber.

Conclusion:

This idea aligns closely with research on developing sustainable thin-film solar cell technology. By increasing the efficiency and practicality of large-scale Cadmium Telluride solar panels, this study offers new insights. This could help bridge the gap between current material limitations and the growing global demand for renewable energy [4,11,22]. This study assists in producing a CdTe solar cell module on a big scale because Telluride is not a readily available element. This study presents a CdTe solar cell to achieve a high efficiency of 27.7% using only 2 µm. The device was studied using SCAPS-1D computer simulations. The absorber materials can absorb different parts of sunlight, which helps improve the current and voltage of the solar cell while using less material [22]. The study also optimised important factors such as absorber thickness, doping concentration, and window-layer thickness. The simulations showed that the absorber cell performs better at higher temperatures and loses efficiency more slowly. These results suggest that the CdTe structure could be useful for developing thin, efficient,

low-cost, and scalable solar cells. However, experimental studies are still needed to confirm its stability and the quality of the interface between the two absorber layers [25].

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Data Availability:

The authors declare that new data were generated or analysed in this study, and they were made available to all.

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