In silico process modeling of effect of MoTe2 as hole transport layer in CuSbS2 absorber based solar cells using SCAPS-1D software

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Research Article

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Abstract

Copper antimony sulphide ($CuSbS_2$) is a suitable material for construction of solar cells as an absorber, since it increases absorption of solar radiation in cells, and hence energy generation. Another material, $MoTe_2$, which acts as a hole transport layer (HTL) is also preferred for solar cells design. $MoTe_2$ HTL provides an addition back surface field that increases the collection of holes at back contact, thus facilitating generation of photonic energy. The presented research involves an *in-silico* examination of their tandem effect in solar energy generation, using the simulation software SCAPS-1D. Results reveal that in the $MoTe_2$ HTL solar cells having 2500 nm thickness of $CuSbS_2$ absorber layer, the maximum power conversion efficiency achieved was 30.4%, at a bandgap of 1.4 eV. The effects of energy bandgap and thickness of $CuSbS_2$ absorber layer on performance parameters of solar cells containing short-circuit current (J_{sc}), open-circuit voltage (V_{oc}), and fill factor (FF) were also studied. Further, effect of operating temperature was also examined to analyse feasibility on outdoor installation of the designed solar cell.

1. Introduction

Solar cells are one of the most promising and well-known means of generating renewable energy. These cells can absorb solar radiation, and convert that to electrical impulses (energy) by the photovoltaic effect (PVE). This process is quick, non-cumbersome, cost effective, safe and environmentally benign.

The process efficiency of solar energy generation depends largely on type of material employed in the construction of such solar panels. Among many material choices available, copper antimony sulphide ($CuSbS_2$), a member of the class of chalcogenide absorber material, is suitable for photovoltaic cells. The said material sufficiently absorbs incoming solar radiation, and aids in PVE. The material is also eco-friendly and economical. The bandgap reported for the said material is between 1.38–1.65 eV [1–3], and it also has an absorption coefficient $> 10^5$ cm^{-1} [1]. These attributes favour absorption of photonic energy. However, to achieve maximum efficiency, certain enhancements are done on the original material, such as the chemical bath deposition (CBD). The CBD method is used on the native material that produces efficiency at 0.66% [4]; whereas, planar heterojunction based solar cells with same material have an efficiency at 0.68% [5]. The present work involves $CuSbS_2$ as the absorber layer for incoming solar radiation.

Besides the core construct material, the hole transporter layers in solar cells also have significant role on the cells' functionality. In perovskite solar cells, $CuSbS_2$ has reportedly been used as hole transport layer to achieve an efficiency of 23.14% [6]. In another find, lead free $MASnI_3$ based solar cell with $CuSbS_2$ as hole transport layer attained an efficiency 24.1% [7].

To further build upon the performance of solar cells, transition metal dichalcogenides (TMD) monolayer are used, wherein M is transition metal type atom (Mo, W) and X is chalcogen metal type atom (S, Se, Te). They are the thin MX_2 type semiconductor materials. In such fabrication, single M transition atoms layers are sandwiched between two X chalcogen atom layers. It then develops attractive and unique properties, such as high carrier mobility and fast charger transfer potential, which have applications in optoelectronic and electronic devices. For such purposes, molybdenum telluride is an appropriate compound of molybdenum and tellurium ($MoTe_2$). $MoTe_2$ is used as hole transport layer to improve the electrical devices' performance having solar cells. The $MoTe_2$ layer is at the interface between 'Mo' back contact and the absorber layer.

In the present *in-silico* work, variation in absorber layer ($CuSbS_2$) bandgap, thickness of $CuSbS_2$ absorber and operating temperature have been evaluated with respect to energy efficiency, using SCAPS 1-D software. The said software is quite reliable and has been employed in many publications already involving solar cells, such as for performance evaluation of solar cells constructed with TiO_2/CuO [8], and also in one of previous publications on performance evaluation of solar cells with $CuSbS_2$ as solar cell construct material [9]. The data between with $MoTe_2$ hole transport layer and without hole transport layer have been subsequently compared for a comparative study. The study aims to investigate the effects of involving a hole transport layer in solar cells, with an absorbed material.

2. Materials And Methods

2.1 Materials

A multi-layered sandwiched structure as a solar cell construct was envisaged in the present work. The composite microstructure was expected to gain in enhanced energy production. The schematic multi-layered sandwiched structure of the solar cell with layers of different metal composites has been shown in Fig. 1.

The said figure shows the front contact face of the cell, beginning from top with n-type ZnO (200 nm), n-type layer CdS (80nm), p-type layer $CuSbS_2$ (1000nm), p-type layer $MoTe_2$ (20 nm), and finally back contact at the bottom. The n-type ZnO, n-type CdS, p-type $CuSbS_2$, and p-type $MoTe_2$ act as window layer, buffer layer, absorber layer and hole transport layer, respectively. The material parameters that have been considered in the present simulation exercise have been referred from literature (Table 1).

Table 1
Electrical and optical properties of materials from literature

Parameters (Unit)	Different layer of solar cell			
	ZnO^*	CdS^*	p-$CuSbS_2$*	p-$MoTe_2$ #
Thickness (nm)	200	80	2500	20
Band gap edge (eV)	3.37	2.41	1.45	1.29
Electron affinity (eV)	4.5	4.2	4.5	4.2
Permittivity	9	9	3.43	13
Density of state, N_C (cm^{-3})	$2.2x10^{18}$	$2.2x10^{18}$	$1.23x10^{20}$	$4x10^{16}$
Density of state, N_V (cm^{-3})	$1.8x10^{19}$	$1.8x10^{19}$	$1.78x10^{20}$	$3x10^{18}$
Electron thermal velocity (cm/s)	10^7	10^7	6.8x107	10^7
Hole thermal velocity(cm/s)	10^7	10^7	$6.07x10^7$	10^7
Mobility of electrons (cm^2/V_s)	150	160	4	110
Mobility of holes ($cm^{2/}V_s$)	25	50	4	426
Acceptor concentration (cm^{-3})	0	0	$5x10^{17}$	$1x10^{19}$
Donor concentration (cm^{-3})	$1x10^{18}$	$1x10^{18}$	0	0
[9]*, [10]#.				

2.2 Methods

2.2.1 Types of solar cells constructed

Two solar cell structures were evaluated, one with $MoTe_2$ HTL, and another without HTL. In the experiments, temperature exposure of the solar cells was varied from 300 K to 400 K, at an interval of 20 K each.

2.2.2. In silico simulation based experiments on solar cells performance with variable parameters using SCAPS 1D software

For simulation experiments, the present study employed SCAPS (Solar Cell Capacitance Simulator) software package, a 1-D solar cell simulation program (Version 3.3.07) developed at University of Ghent, Belgium by Dr. Marc Burgelman [11]. The software is aptly suited to meet the simulation needs of variety of solar cell based objectives.

It can simulate up to seven layers structure device. The objective was to assess the effect of various layers on overall performance of the solar cell, and to understand the methods to optimize such efficiency. The data obtained has been subjected to graphical representation to illustrate the performance indices.

2.2.3 Statistical analysis

To test statistical significance of data (experimental vs. reported), students t-test at $p \leq 0.05$ using MS-Excel (Microsoft Corp., USA) was conducted.

3. Result And Discussion

3.1 Effect of variation of band gap on $CuSbS_2$ absorber in solar cells

The present study indicated that the $CuSbS_2$ absorber layer's band gap varied from 1.0 eV to 1.8 eV, at the interval of 1.2 eV. All the performance parameters have been depicted in Fig. 2. In Fig. 2(a), 'V_{oc}', and in Fig. 2(c) 'field factor' of solar cell with HTL $MoTe_2$ showed an increase in the band gap of absorber layer, with an increase up to 1.4 eV that saturated thereafter. However, V_{oc} increased for all values of band gap values of the absorber, even without HTL solar cell. Figure 2(b) indicated that short circuit current (J_{sc}) decreased with increase in band gap of absorber layer for structure of the solar cell.

The power conversion efficiency (PCE) of both solar cells increased, up to band gap of 1.4 eV; but, any further increase in band gap caused PCE to decrease. This observation could be owing to fewer electron moving from valence to conduction band. This process has been schematically depicted also [Figure 2(d)]. The highest power conversion efficiency with HTL was 27.87% (V_{oc} = 0.97 V, J_{sc} = 34.1 mA/cm^2 and %FF = 84.08%), and without HTL was 20.96% (V_{oc} = 0.89 V, J_{sc} = 28.07 mA/cm^2 and %FF = 83.20%). The optimized PCE at about 28% was at band gap 1.4 eV with HTL (Fig. 2d).

3.2 Effect of variation of thickness of $CuSbS_2$ absorber in solar cells

In this part of the work, $CuSbS_2$ absorber layer thickness was varied from 500 nm to 2500 nm, at an interval of 500 nm. All performance parameters, as in previous section of study, were also adopted herein, and have been depicted in Fig. 3. Figures 3 (a) and (c) show that V_{oc} and FF, when without HTL, increase for all value of thickness of absorber layer. But, with HTL these values decreased for all values of absorber layer, with reduced thickness of panel material.

Figures 3 (b) and (d) show that values of J_{sc} and PCE, with HTL and without HTL, increased for all values of the absorber layer. The highest conversion efficiency of absorber layer with $MoTe_2$ HTL was 30.4% (V_{oc} = 1.00 V, J_{sc} = 36.08 mA/cm^2, %FF = 84.02%); while without HTL, highest power conversion efficiency was

25.89% (V_{oc} = 0.97 V, J_{sc} = 31.60 mA/cm^2, %FF = 84.31). Thus, HTL increased efficiency of the solar cells, with optimized value at 2250 nm, with PCE at 30% (Fig. 3d). This observation could be owing to the fact that the HTL blocked electrons, and provided passage to the holes emanating from the depletion region. HTL also reduces the carrier recombination of the back contact solar cell.

When the value of thickness of the absorber layer increased, longer wavelength photons were absorbed in the said layer that generated additional number of electron hole pairs. Hence, values of V_{oc} and J_{sc} also increased. Thickness in solar cells is also debated at length. Few opine that thickness, even though improves performance of the solar panel, such thick cells may experience higher recombination rates. Since recombination represents loss of energy of electrons such that they drop from conduction band to valence band. Thus, opposed to photogeneration, a higher than threshold thickness may not be useful. It should be such that generation rate > recombination rate so that sufficient carriers are available to carry the photocurrent in the solar cell [12].

3.3 Effect of variation of temperature on $CuSbS_2$ absorber

The performance of the composite cell under temperature stress has been interesting. All the performance parameters have been depicted in Fig. 4. The Figs. 4 (a, c, d) depict that fill factor and PCE values decreased for both constructs of solar cells. Figure 4(b) illustrates that 'J_{sc}' slightly increased with increase in temperature because band gap energy slightly decreased therein. This created extra energy photons to produce electron hole pairs under such circumstances. The highest power efficiency with HTL was 27.32% (V_{oc} = 1.01 V, J_{sc} = 31.87 mA/cm^2, %FF = 84.71). The same without HTL power conversion efficiency was 20.88% (V_{oc} = 0.94V, J_{sc} = 26.28 mA/cm^2, %FF = 84.03) (Fig. 4d).

In agreement with our data, it is notable that low temperature operation has also been typically favoured for solar cells in other studies as well. Improved performance of solar cells at low temperatures has been observed for TiO_2/CuO solar cells [8]. With increase in temperature, the band gap of the semiconductor material of the solar cell becomes reduces, causing fall in V_{oc}. The decreased voltage is owing to dependency of p-n junction on temperature. This causes lesser release of charged particles at the same intensity of incident solar radiation, resulting in drop in energy generation. However, the current increases, due to the fact that more number of electrons are raised from valence band to conduction band, causing increased photocurrent [13].

The increased current at high temperature has also been reasoned on the basis that more than necessary energy is available to excite electrons in semiconductor for PVE to occur. The increased concentration of electrons at high operating temperatures increases carrier current, as voltage in solar cell drops [14]. Typically, any solar module would operate between 20–40°C (293–313 K), depending on the design and intensity of incoming sunlight. This type of temperature situation in the open is quite critical in tropical countries (ambient temperature 30–40°C) for solar panel installation, and appropriate operational care must be taken for adequate efficiency, given the temperature effects discussed. .

Excessive increases in temperature can also damage the cell and other module material. This phenomenon is well explained by Al-khazzar. The author points out that due to increased electrical resistance at high temperatures in conducting materials, mobility of charged carriers (electrons) decreases, and as a result voltage drops. This phenomenon is also justified by the fact that carrier mobility is inversely related to temperature [15]. Hence, our finding is in unison with the concept of low temperature performance for solar cells.

Similar findings on improved solar cells performance with multi-layered composite has also been reported by other authors as well. It has been empirical proven that fabrication of parent solar cell construct with additional materials is a success. Spray based solar cell with $CuSbS_2$ (as an absorber layer) has been fabricated to achieve maximum power conversion efficiency at 0.34% [16]. Also, Ag-substituted thin film solar cell reportedly improves the efficiency from 0.73–2.48% [17]. In another find, researchers obtained $CH_3NH_3GeI_3$ perovskite solar cells based on $CuSbS_2$ with efficiency ~ 2% [18]. Selenized $CuSbS_2$ improves the device performance efficiency 0.78% [19]. These data strongly suggest constructive role of $CuSbS_2$ in solar power generation.

3.4. Performance indices of solar cells with HTL

The performance data of photovoltaic parameters of solar cells with HTL and without HTL, as observed experimentally have been presented in Table 2. The data has also been compared with a similar work on $CuSbS_2$ as solar absorber, but without HTL. Comparing common performance indices, it is evident that statistically significant difference of solar cells with HTL and without HTL occurred for all test parameters except fill factor. Also, for solar cells without $MoTe_2$, statistically insignificant difference between cells of present study without HTL and a similar work conducted by Sadanand and Dwivedi of our research group previously, confirming correct cells construct in the present work, and compliance of material qualities [9]. This observation further establishes reliability of data obtained with $MoTe_2$, with regards material quality and attributes.

Table 2

Comparison of photovoltaic parameters of solar cells with HTL and without HTL

Thickness of $CuSbS_2$ absorber layer	HTL ($MoTe_2$)	Open –circuit voltage, V_{oc} (V)	Short circuit current density, J_{sc} (mA/cm^2)	Fill factor, FF (%)	Power conversion efficiency, PCE (%)
1000 nm*	Not used*	0.91 ± 0.02 [a,*]	28.25 ± 1.80 [a,*]	81.10 ± 2.50 [a,*]	21.09 ± 1.90 [a,*]
1000 nm	Not used	0.94 ± 0.02 [a]	26.28 ± 1.90 [a]	84.03 ± 2.30 [a]	20.88 ± 1.80 [a]
1000 nm	$MoTe_2$	1.01 ± 0.01 [b]	31.87 ± 2.10 [b]	84.71 ± 2.60 [a]	27.72 ± 1.85 [b]
[9]*.					
[a,b]Different letters in a column represent significant difference at $p \leq 0.05$.					

Evidently, significant increase in parameter values such as V_{oc}, J_{sc}, %FF and %PCE confirm a constructive role of $MoTe_2$. Using p-$MoTe_2$ few authors have achieved efficiency of solar cells as high as 16%, at HTL thickness at least 60 nm, when working on CdTe film as solar panel material. The said experiments were also in silico, being a simulation product of SCAPS 1D software [20]. Another similar experiment using HTL in Sb_2Se_2 (absorber) in solar cells with CuO as HTL material has been a success. The said experiment also involved SCAPS-1D simulation software, and reported a 23.18% efficiency [21]. In fact, the congruence of simulation data of SCAPS 1D in solar cells with testimony from empirical experiments has been evident in formamidinum perovskite solar cells [22], justifying possible similarity of the simulation data obtained in the present work, with experimental data (when conducted).

4. Conclusion

In the present work, a simulation based *in silico* experiment was conducted involving the $ZnO/CdS/CuSbS_2/MoTe_2$ multilayered structured device for solar power generation with photovoltaic effect. Different parameters affecting the performance of solar cell were examined. $MoTe_2$ that was used as hole transport layer, achieved a promising result, with values of %PCE (27.72), with V_{oc} (1.01 V), J_{sc} (31.87 mA/cm^2) and %FF (84.71). These data suggest constructive role of $MoTe_2$ as a hole transport layer in solar cells with $CuSbS_2$ as absorber layer for better performance.

Declarations

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Data availability: The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request

Declaration of Interest: The authors declare no competing interest

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Figures

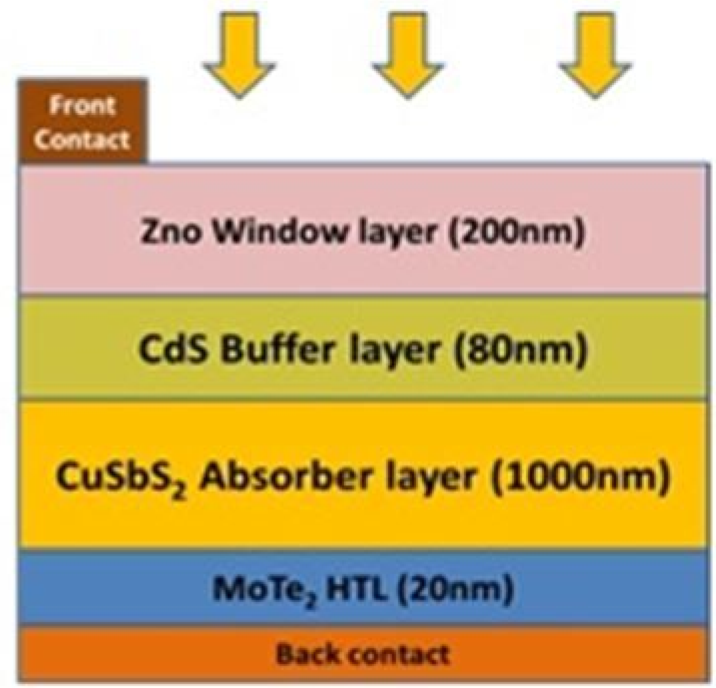

Figure 1

Device structure of CuSbS2 based solar cell.

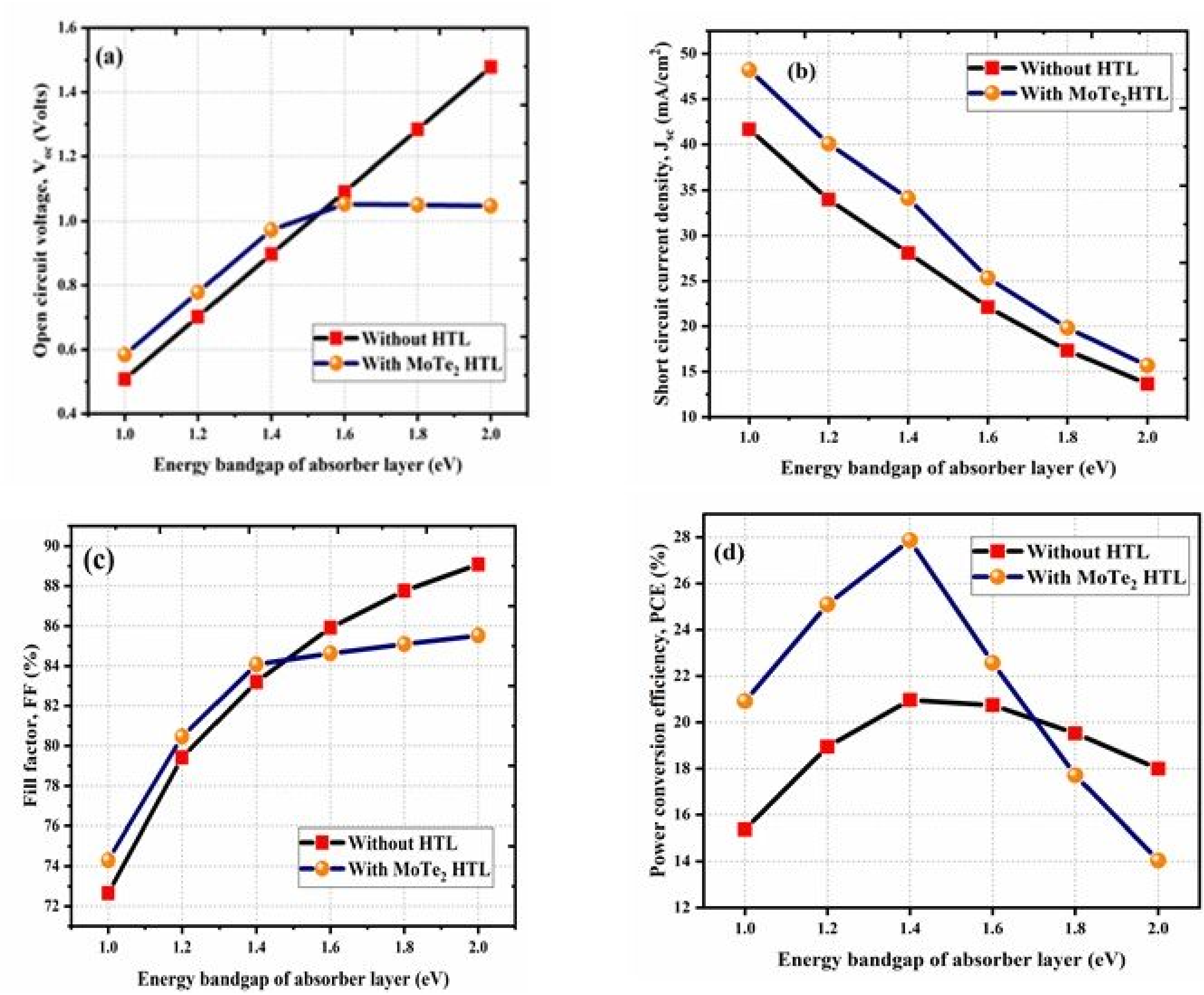

Figure 2

Effect of device performance of band gap variation CuSbS2absorber layer solar cell (a) Open circuit voltage (V) (b) Short circuit current density (mA/cm2), (c) Fill factor (%) (d) Power conversion efficiency (%).

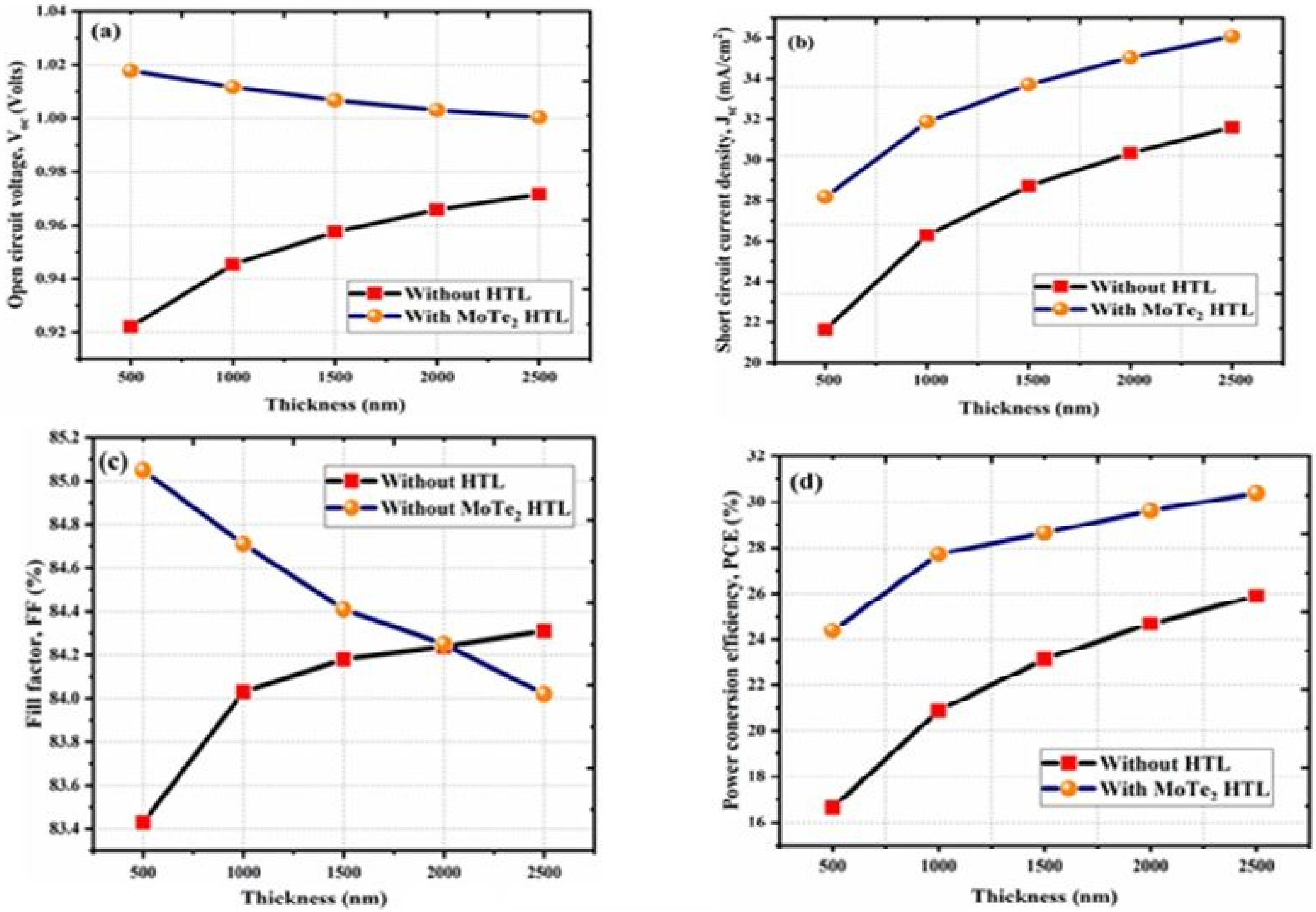

Figure 3

Effect of device performance of thickness variation CuSbS2absorber layer solar cell (a) Open circuit voltage (V) (b) short circuit current density (mA/cm2) (c) Fill factor (%) (d) Power conversion efficiency (%).

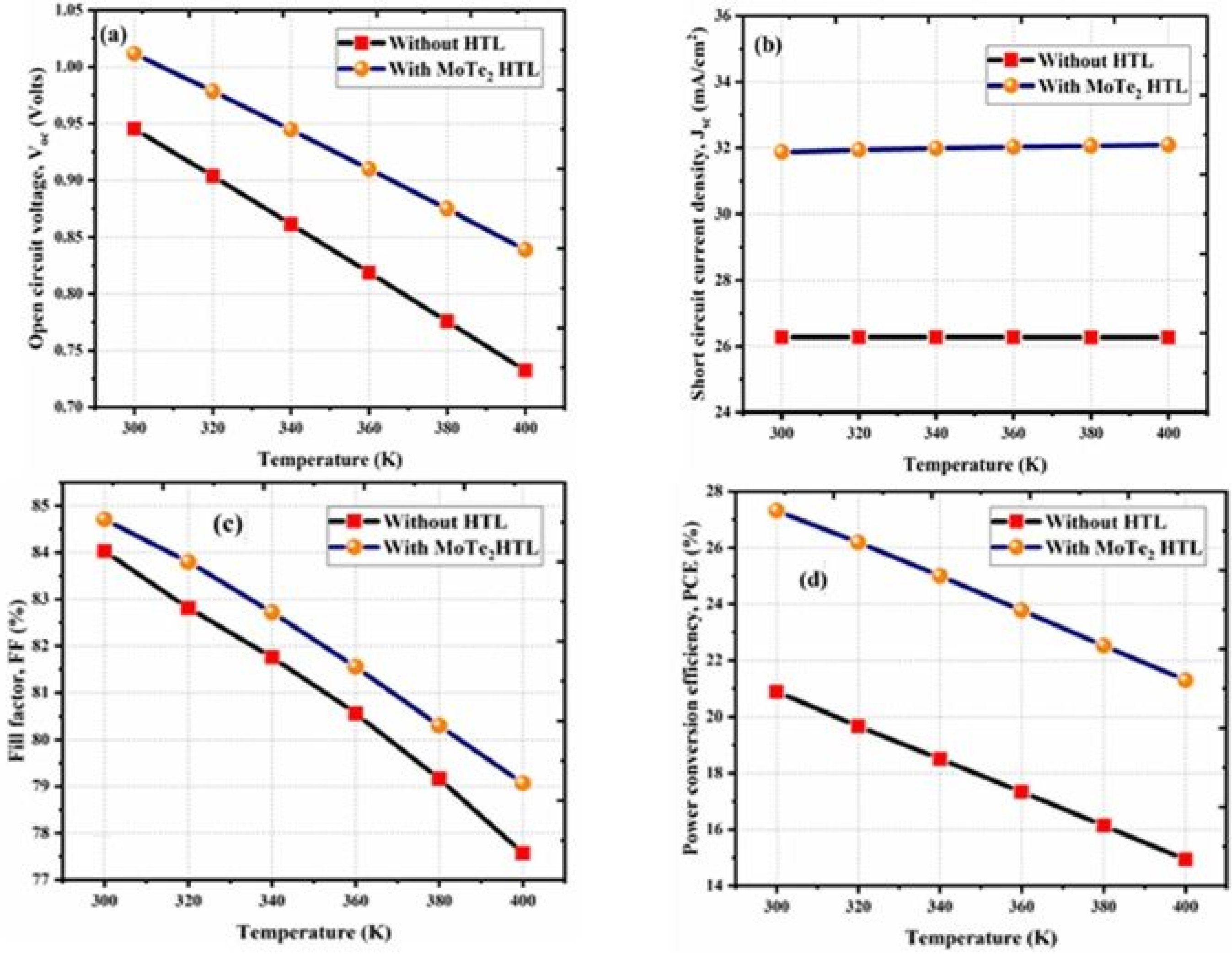

Figure 4

Effect of temperature variation of solar cell (a) Open circuit voltage (Voc) (b) Short circuit current density (Jsc) (c) Fill factor (%) (d) Power conversion efficiency (%).