Numerical simulation for optimization of ultra-thin n-type AZO and TiO₂ based textured p-type c-Si Heterojunction Solar Cells

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Research Article

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Abstract

A maximum efficiency of 17% for ultra-thin n-type AZO layer and 17.5% for ultra-thin n-type TiO_2 layer based silicon heterojunction solar cell is reported by optimizing its properties which is much higher than practically obtained efficiency signifying a lot of improvements can be performed to improve efficiency of TiO_2/Si and AZO/Si heterojunction solar cell. AZO layer and TiO_2 layer is used as n-type emitter layer and crystalline silicon wafer is used as p-type (p-cSi) layer for modelling AZO/Si and TiO_2/Si heterojunctions solar cell respectively using AFORS HET automat simulation software. Various parameters like thickness of AZO, TiO_2 layer, p-cSi layer, doping concentration of donors (Nd) and effective conduction band density (N_c) are optimized. Finally, texturing at different angle is studied and maximum efficiency is reported at 70 μm thick p-type crystalline Silicon (p-cSi) wafer, that can be very helpful for manufacturing low cost HJ solar cells at industrial scale because of thin wafer and removal of additional processing setup required for deposition of amorphous silicon i-layer. Utilization of TiO_2 and Aluminium doped Zinc Oxide as n-type layer and p-cSi as p-type layer can help in producing low cost and efficient heterojunction (HJ) than compared to HJ with intrinsic thin layer HIT solar cells.

Introduction

Demand of energy consumption is tremendously increasing day by day in today's world and to meet the same, contribution from renewable energy sources has to be increased. Conventional non-renewable energy sources are limited and have many environmental concerns. Renewable energy sources are the solution to overcome the problems related to non-renewable energy sources like pollution, limited stock, environmental problems, etc. [1]. In recent times, solar energy is one of most widely commercially used renewable energy source. Photovoltaic solar cell technology is currently dominated by silicon wafer based solar cells by almost 90% [2]. In recent past, silicon heterojunction solar cells developed by sanyo company based on heterojunction with intrinsic thin layer (HIT) concept is widely used to manufacture solar cells at industrial scale due to their good efficiency, cost effectiveness and economic viability [3, 4]. Further, numerous research on thin film based silicon heterojunction solar cell is ongoing using metal oxides as n-type layer with crystalline silicon (p-cSi) wafer as p-type as well as metal oxides as p-type layer with n-type cSi (n-cSi) wafer due to their easy availability and environment friendly [5–9]. Aluminium doped zinc oxide (AZO) and zinc oxide can be used as window layers, antireflection coating (ARC) layer & as TCO layer in solar cells [10, 11]. They also find applications in other devices like transducers, ultrasonic oscillators and gas sensors. ZnO can be used as a substitute for indium tin oxide (ITO) as it is cheaper than ITO and also enhances the efficiency of solar cells [12]. ZnO can be doped with elements like Al, B, F, Ga, In etc. to make it n-type ZnO. Titanium dioxide (TiO_2) can also be used as n-type layer which has significant electrical conductivity and high visible transparency [13]. TiO_2 can be doped to make further n-type or p-type material, where it can be doped with Cr^{3+} , Fe^{3+} , Ni^{+2} and Co^{+2} to make p-type and elements like Sn, N, Al, F etc. to make n-type TiO_2 . TiO_2 can be fabricated using physical and chemical deposition techniques. Some vacuum based techniques like sputtering, pulsed laser deposition (PLD), chemical vapour deposition (CVD) and some solution based techniques like sol-gel, dip/spin coating, and spray

pyrolysis can be used for deposition of TiO_2 films. Vacuum based technology is used for fabrication of solid state device, although this technology is more expensive than solution based technology. Sputtering method is suitable for uniform coating on substrate with large area. It has been established as standard technique for deposition of transparent semiconducting oxide films. Pulsed laser deposition (PLD) technique is used for deposition of robust and nanostructured thin films. This technique is very efficient technique which is capable to assist laser desorption and ionization of low molecular weight. Chemical vapour deposition (CVD) offer various advantages over other techniques like purity of thin film, low cost than compared with other vacuum based technology, thin film with different morphology and good adhesion with substrate [13]. Although, sol-gel technique is not suitable to produce TiO_2 thin film for solar cell application, they offer other advantages like compositional control, homogeneity and low crystallization temperature [13]. Spray pyrolysis offers advantages like low cost, scalable and uniform deposition on large area substrate. TiO_2 thin film in its pure form, without doping has low conductivity that makes them unsuitable for solar cell application where doped TiO_2 layer can be used to make them suitable for photovoltaic [14, 15]. However, practical efficiency is very low for such solar cells due to various defects and improper optimization of parameters. Their various parameters can be optimized using various numerical simulation softwares like PC1D, AFORS-HET [16], silvaco ATLAS [17, 18], TCAD [19, 20], AMPS [21], SCAPS 1D [22–24] etc. AFORS-HET is an automat simulation software based on Shockley-read-hall recombination statistics which solves one-dimension semiconductor equation [7, 25, 26]. This software is used for modelling homojunction and heterojunction devices [25, 27, 28]. This program solves 1-D semiconductor equation which is based on physical differential equation like transport & continuity equation and poisson's equation [29]. Lambert beer law is used which is based on optical model for estimation of optical parameter [7]. In this work, AFORS-HET automat simulation software is used to simulate AZO/Si and TiO_2 /Si heterojunction solar cell and its various parameters like thickness of silicon wafer, thickness of AZO layer, thickness of TiO_2 layer, doping concentration of donors (N_d), effective conduction band density (N_c), and texturing at different angle is optimized [30]. Texturing of silicon wafer at different angle is performed to study the change in behaviour and performance of solar cell with respect to plane heterojunction solar cell [31, 32]. Texturing plays important role for improvement in performance of thin film based silicon heterojunction solar cells due to increment in light trapping of incoming light and multiple internal reflection, which helps to increase charge carrier transport and hence, enhances the overall efficiency of solar cell [33, 34]. Various literatures are reported for plane and textured (pyramidal and inverted pyramidal) solar cells [35, 36]. Efficiency is also dependent at various texturing angle and hence, desired texturing angle can be applied to produce maximum power conversion efficiency from solar cell [37]. Using AZO as n-type material, an efficiency of 6.8% is reported for Al:ZnO/CdS/CuInSe₂ polycrystalline solar cell in [10]. 6.8% efficiency is reported for Al:ZnO/Si heterojunction solar cell in [38]. However, maximum theoretical efficiency of 29.43% can be achieved for silicon heterojunction in [39–41] respectively. A maximum efficiency of 17% for ultra-thin n-type AZO layer and 17.5% for ultra-thin TiO_2 as n-type layer is achieved by optimizing its properties which is much higher than practically obtained efficiency signifying a lot of improvements can be performed to improve efficiency of TiO_2 /Si and AZO/Si heterojunction solar cell.

Simulation Details And Device Structures

AFORS-HET automat simulation software is used in this work for modelling the AZO/Si and TiO₂/Si heterojunction solar cell where ultra-thin AZO layer & TiO₂ layer acts as n-type layer and crystalline p-type silicon (p-cSi) wafer acts as p-type absorber layer. Device structure used for modelling in this work is described in figure 1. All default values present in AFORS-HET software are considered for the modelling TiO₂ & AZO layer based silicon heterojunction (SHJ) solar cells except the parameters used to be optimized. Illuminance of radiation AM 1.5 is used with power density of 100 mW/cm² for simulation in present study. Standard values of Al:ZnO, TiO₂ and p-cSi are taken from references [7, 15, 25]. Flatband schottky front interface and flatband schottky back interface is chosen as default in present study. No interface effect is studied in this article, hence 'No Interface' is considered as default. Front contact boundary and back contact boundary are chosen as constant (zero) i.e. no absorption loss is considered. Carrier lifetime in silicon is considered as 1 msec; Diffusion length of carriers in silicon wafer is considered to be around 100 µm. Resistivity and order of series resistance and shunt resistance of layer has been taken as default values i.e. minimum for series resistance (R_s : 0 ohm) and max for shunt resistance (R_{shunt} : 10³⁰ ohm). In this work, following studies are carried out: (i) thickness optimization of p-cSi layer, (ii) thickness optimization of ultra-thin AZO and TiO₂ layer, (iii) optimization of doping concentration of donors (N_d), (iv) optimization of effective conduction band density (N_c) and (v) optimization of texturing at various angles.

Table 1 Input parameters used for AFORS-HET numerical simulation with p-type crystalline silicon wafer as p-layer and AZO &TiO₂ as n-layer.

Parameter		p-cSi	AZO	TiO ₂
Thickness	d	varied (μm)	varied (nm)	varied (nm)
Dielectric Constant	dk	11.9	9	8.6
Electron Affinity	eV	4.05	4.4	3.9
band gap	eV	1.12	3.37	3
Opt. BG	eV	1.12	3.3	3
Effective CB density	cm ⁻³	varied	varied	varied
Effective VB density	cm ⁻³	2.5×10 ¹⁹	1×10 ¹⁹	1×10 ¹⁹
Electron mobility	cm ² V ⁻¹ s ⁻¹	1041	100	20
hole mobility	cm ² V ⁻¹ s ⁻¹	412.9	25	10
Acceptor concentration	cm ⁻³	1.5×10 ¹⁶	0	0
donor concentration	cm ⁻³	0	varied	varied
Thermal vel. of e	cms ⁻¹	1×10 ⁷	1×10 ⁷	2.99×10 ⁶
Thermal vel. of h	cms ⁻¹	1×10 ⁷	1×10 ⁷	6.76×10 ⁶
layer density	gcm ⁻³	2.328	2.33	2.328

Texturing plays important role in enhancing the efficiency of solar cells [33]. Texturing of silicon wafer surface can be performed through chemical etching. Due to textured morphology of layers in solar cells there is re-absorption of reflected rays which helps in minimizing the lost reflected light [12]. Texturing increases excess charge carriers due to light trapping and multiple internal reflection which helps in enhancing overall performance & conversion efficiency of solar cell. Moreover, efficiency also depends on angle at which texturing is performed to produce an efficient solar cell [42]. There are several reports on pyramidal and inverted pyramidal texturing for silicon solar cells [12, 33]. In this article, texturing is performed at various texturing angle and performance of modelled AZO/Si heterojunction solar cell is optimized.

Results And Discussion

1 Thickness optimization of p-cSi silicon wafer:

In this section, thickness of p-type crystalline silicon wafer is optimized. Manufacturing of solar cells using thin p-cSi wafer can be cost effective up to certain extent at industrial scale. Though nowadays n-cSi ingots are also reasonable in cost compared to p-cSi and wafer of around 200 μm thickness are in

use at industrial scale. However, through our simulation we have obtained that its thickness can further be reduced to upto 70 μm without affecting its performance. All other parameters were in accordance with the values reported in Table-1. Efficiency rapidly increases with thickness initially, begins to saturate after 70 μm and remains constant upto 500 μm . This can be well explained as initially as thickness increases, more number of charge carriers are generated and contribute to flow of charge across p-n junction. However, after certain thickness, charge carriers generated does not travel across junction due to thickening of wafer and less diffusion length of charge carriers in silicon wafer which is around 100 μm . When thickness of silicon wafer gets thicker than its diffusion length, charger carriers generated does not travel upto p-n junction and gets recombined and hence charge carriers generated having diffusion length more than 100 μm does not participate in charge collection. Thus, efficiency begins to saturate after 70 μm . Also, film gets flexible when its thickness reduces beyond 50 μm . Experimentally, an ultrathin flexible film of thickness 45 μm has been fabricated by [43] using Cu-assisted chemical etching of bulk c-Si producing conversion efficiency of over 17%. Also, mechanical stress, multi flexure, fracture and static test has been conducted by [44] for flexible thin films based crystalline silicon solar cells where thickness of flexible thin film varying from 20 μm to 50 μm . Thus, an ultrathin stable film can be utilized for silicon based HJ solar cells. Hence, the thickness of p-type silicon wafer at 70 μm is optimized in this work. Similar pattern is also observed for short circuit current (J_{sc}) curve. This behaviour is well illustrated in V_{oc} vs thickness curve **figure: 2(a)**, J_{sc} vs thickness curve **figure: 2(b)** and fill factor (FF) vs thickness curve **figure: 2(c)**. V_{oc} , J_{sc} and FF values remains nearly constant from 70 μm to 500 μm ; V_{oc} and J_{sc} rapidly decreases on further reducing the thickness of p-cSi layer which accounts for the decrease in efficiency. Fill factor firstly increases slightly and then decreases but this increase is less significant than rapid decrease in V_{oc} and J_{sc} which results in decrease in efficiency. Hence, the thickness of p-cSi layer is optimized at 70 μm to obtain an efficiency of 12.84% for AZO layer and 12.16% for TiO_2 layer based p-cSi HJ solar cells.

2 Thickness optimization of ultra-thin n-type AZO and TiO_2 layer:

Thickness of AZO and TiO_2 layer is varied from 0.5 nm to 10 nm and open circuit voltage (V_{oc}), short circuit current (J_{sc}), fill factor (FF) and efficiency is recorded with respect to thickness of AZO & TiO_2 layer, Figure 3 (a) to (d) represents curve for each respectively. All other parameters were in accordance with the values reported in Table-1. There is no effect of thickness variation of TiO_2 layer on V_{oc} and it remains constant at 546.1 mV. Same pattern is observed for AZO layer as well, However, there is slight enhancement in V_{oc} at 3 - 4 nm, giving maximum V_{oc} of 549.2 mV below 3 nm. Short circuit current linearly decreases with increase in its thickness giving maximum J_{sc} at 0.5 nm. However, due to practical limitations, deposition of layers using modern techniques is limited upto 3 nm for stable film and hence J_{sc} at 3 nm giving short circuit current of 29.12 mA for ultra-thin AZO layer and 29.02 mA for ultra-thin TiO_2 layer based solar cell is considered as optimized short circuit current [7]. This behaviour is expected, since thinning of emitter layer will contribute to flow more number of charge carriers generated in absorber layer and easy transport across layer due to decrease in resistance, thus recombination rate also

decreases; hence resulting in enhancement of short circuit current with decrease in thickness of emitter layer. Fill factor also decreases linearly with increasing thickness. This can be attributed due to decrease of series resistance as we decrease its thickness. Hence, overall efficiency increases linearly with decreasing thickness and gives maximum efficiency of 12.84% for ultra-thin n-type AZO layer and 12.59% for ultra-thin n-type TiO_2 layer based HJ solar cell.

3 Doping concentration of donors (N_d)

Doping of donor concentration plays an important role in enhancing the charge carriers which resulted in improved efficiency. Figure 4 (a) to (d) represents the variation of V_{oc} , J_{sc} , FF and efficiency curve with respect to doping concentration of donors respectively, where N_d is varied from 10^{14} cm^{-3} to 10^{18} cm^{-3} . Doping can be achieved in order of 10^{20} cm^{-3} using various techniques like ion implantation, mixed molecular monolayer doping technique etc. [45]. Introduction of doping concentration of donors doesn't affect open circuit voltage (V_{oc}) much and it nearly remains constant for both, AZO and TiO_2 layer excluding for TiO_2 at lower concentration. Short circuit current (J_{sc}) effectively decreases with increase of doping concentration of donors, giving maximum short circuit current of 30.1 mA and 30.3 mA for AZO and TiO_2 layer respectively. Maximum fill factor at 10^{15} cm^{-3} for TiO_2 layer and at 10^{16} cm^{-3} for AZO layer is observed and it nearly remains unaffected on further increasing doping of donors. Similar pattern is followed in efficiency curve as well, where maximum efficiency of 13.13% for AZO layer and 13.21% for TiO_2 is reported at doping concentration of $1 \times 10^{15} \text{ cm}^{-3}$ and $1 \times 10^{14} \text{ cm}^{-3}$ respectively. Performance of device degrades as doping concentration increases beyond order of 10^{15} which can be due to introduction of defect states in AZO and TiO_2 layer at higher doping concentration limiting its performance. With increase in defect states in space charge region, it can create conduction channel across it and leakage current starts flowing which degrades the performance of device. Hence, efficiency decreases with further increase of doping concentration for AZO layer beyond 10^{15} cm^{-3} . Similar pattern is followed for TiO_2 layer as well, where efficiency remains nearly constant upto 10^{15} cm^{-3} and decreases thereafter due to introduction of defect states at higher concentration.

4 Effective conduction band density

During carrier charge transport, effective conduction band density and effective valence band density are the major density of states that plays important role during charge transport. Figure 5.1 to 5.4 represents the variation of V_{oc} , J_{sc} , FF and efficiency curve with respect to effective conduction band density respectively. All other parameters were in accordance with the values reported in Table-1. Effective conduction band density is varied from 10^{15} cm^{-3} to 10^{19} cm^{-3} as shown in **figure 5(a) to 5(d)**. Similar variation in tail density of states from 10^{13} cm^{-3} to 10^{21} cm^{-3} has been reported in [46]. Open circuit voltage remains constant on varying conduction band density for both, AZO & TiO_2 layer. Short circuit current linearly decreases slightly on increasing N_c giving maximum J_{sc} of 30.4 mA at 10^{15} cm^{-3} for TiO_2 layer and 30.08 mA at 10^{19} cm^{-3} for AZO layer based solar cell. Fill factor is significantly influenced with

N_c and thus contributes more to efficiency. Hence, efficiency follows the pattern like fill factor. Efficiency increases initially exhibiting best efficiency at around 10^{16} cm^{-3} and remains nearly constant thereafter which can be attributed to increase in shunt resistance and decrease in series resistance initially thus affecting fill factor of device accordingly. After certain level, there is no significant change in shunt resistance and series resistance with change in effective conduction band density resulting in nearly constant fill factor, thus efficiency also gets saturated. However, initial increase in efficiency is more significant in case of TiO_2 based solar cell than compare to AZO based silicon solar cell and further study needs to be carried out for more fundamental reason behind this. Maximum efficiency of 13.24% for AZO layer and 13.21% for TiO_2 layer at $5 \times 10^{15} \text{ cm}^{-3}$ and $1 \times 10^{17} \text{ cm}^{-3}$ respectively is obtained for AZO/Si and TiO_2 /Si based HJ solar cells respectively.

5 Texturing angle

Efficiency of solar cell can be significantly enhanced through texturing [35]. Many reports are there on pyramidal and inverted pyramid textured silicon wafer solar cell. Texturing angle is varied from 0° to 89° as shown in **figure 6**. V_{oc} increases linearly with texturing angle giving maximum open circuit voltage 555.5 mV at 89° for both, AZO layer based and TiO_2 layer based silicon HJ solar cells. Similar trend is followed in J_{sc} curve giving maximum short circuit current of 37.81 mA and 38.92 mA at 89° for AZO layer based and TiO_2 layer based silicon HJ solar cells. Fill factor nearly remains constant and varies from 80.25% to 80.96% for entire range of texturing angle. Efficiency follows the same curve, giving maximum efficiency of 17% for AZO layer and 17.5% for TiO_2 layer at texturing angle of 89° . Efficiency increases linearly with texturing angle due to increment in close packing density of textured surface which increases the internal multiple reflection of illuminated light and helps to enhance absorption loss, thus contributes in collecting more charge carriers [42]. Thus efficiency of modelled AZO/Si HJ solar cell is significantly increased. Hence all the parameters of TiO_2 , AZO layer and p-cSi wafer layer is optimized to attain maximum efficiency of 17% for AZO/Si and 17.5% for TiO_2 /p-cSi heterojunction solar cells.

Conclusion

Numerical simulation is performed using AFORS-HET software program to achieve a maximum efficiency of 17% and 17.5% for ultra-thin n-type AZO and TiO_2 layer based silicon HJ solar cell by optimizing its various parameters. In this work, thickness of p-cSi wafer is optimized at $70 \mu\text{m}$ to obtain an efficiency of 12.84% for ultra-thin AZO layer and 12.16% for ultra-thin TiO_2 layer based p-cSi HJ solar cells respectively. It is followed by optimizing thickness of ultra-thin TiO_2 and AZO layer at 3 nm to obtain an efficiency of 12.84% for AZO layer and 12.59% for TiO_2 layer based HJ solar cell respectively. Doping concentration of donors (N_d) is optimized at $1 \times 10^{15} \text{ cm}^{-3}$ for ultra-thin AZO layer and $1 \times 10^{14} \text{ cm}^{-3}$ for ultra-thin TiO_2 layer to obtain efficiency of 13.13% and 13.21% for AZO/Si and TiO_2 /Si HJ solar cells respectively.

Effective conduction band density is optimized at $5 \times 10^{15} \text{ cm}^{-3}$ for AZO layer and at $1 \times 10^{17} \text{ cm}^{-3}$ for TiO_2 layer based solar cell and obtained an efficiency of 13.24% and 13.21% respectively. Finally, the role of surface texturing at various angle is studied and reported the maximum efficiency of 17% and 17.5% for AZO and TiO_2 layer based silicon HJ solar cells respectively. Linear increase in efficiency with respect to texturing angle is observed, where efficiency of 14.21% for AZO layer and 14.45% for TiO_2 layer based silicon HJ solar cells for pyramidal surface texturing is obtained. Thickness optimization of p-cSi at 70 μm and removal of intrinsic amorphous silicon layer can be very cost effective for manufacturing AZO/Si heterojunction solar cells at industrial scale for commercial production; as deposition of i-layer a-Si and other similar based HJ solar cells with intrinsic layer involves additional processing setup. Processing of such layers also has some serious environmental & safety issues. Optimization of texturing angle plays a significant role in enhancing the efficiency above 17% for the above modelled HJ solar cell. Hence, efficiency reported using AZO and TiO_2 layer based silicon heterojunction solar cell in this article can be cost effective and efficient solar cell. Such results are encouraging and exciting for practical applications. However, practically it is challenging to texture the silicon wafer at such angle with high accuracy. Lasers can be used to texture silicon surface at such specific angles though such process may cost more. Further investigation on above modelled cell can be performed by introducing intrinsic thin layer, p+ layer, n+ layer and BSF layer to simulate HIT, HITBSF and HIT-BIFACIAL solar cells to further improve the efficiency of solar cell.

Declarations

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Authors Contribution:

Chandan Yadav: Writing original draft, simulation work. **Sushil Kumar:** Conceptualization, review & editing, supervision.

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Tables

Table 1 Input parameters used for AFORS-HET numerical simulation with p-type crystalline silicon wafer as p-layer and AZO & TiO₂ as n-layer.

Parameter		p-cSi	AZO	TiO ₂
Thickness	d	varied (μm)	varied (nm)	varied (nm)
Dielectric Constant	dk	11.9	9	8.6
Electron Affinity	eV	4.05	4.4	3.9
band gap	eV	1.12	3.37	3
Opt. BG	eV	1.12	3.3	3
Effective CB density	cm ⁻³	varied	varied	varied
Effective VB density	cm ⁻³	2.5×10 ¹⁹	1×10 ¹⁹	1×10 ¹⁹
Electron mobility	cm ² v ⁻¹ s ⁻¹	1041	100	20
hole mobility	cm ² v ⁻¹ s ⁻¹	412.9	25	10
Acceptor concentration	cm ⁻³	1.5×10 ¹⁶	0	0
donor concentration	cm ⁻³	0	varied	varied
Thermal vel. of e	cms ⁻¹	1×10 ⁷	1×10 ⁷	2.99×10 ⁶
Thermal vel. of h	cms ⁻¹	1×10 ⁷	1×10 ⁷	6.76×10 ⁶
layer density	gcm ⁻³	2.328	2.33	2.328

Figures

(a)

(b)

Figure 1

represents the designed structure for planar and textured AZO/Si HJ and TiO₂/Si HJ Solar cells used in numerical simulation with different layer where fig (a) represents planar AZO/Si HJ and TiO₂/Si HJ solar cells and fig (b) represents textured AZO/Si HJ and TiO₂/Si HJ solar cells.

Figure 2

The performance of modelled AZO and TiO₂ based silicon HJ solar cell with variation in thickness of p-cSi wafer where Fig (a) – (d) represents V_{oc} , J_{sc} , FF and η vs thickness of p-cSi wafer

Figure 3

The performance of modelled solar cell with variation in thickness of AZO and TiO₂ layer where Fig (a) – (d) represents Voc, Jsc, FF and η respectively w.r.t. thickness of emitter layer.

Figure 4

The performance of modelled solar cell with variation in doping concentration of donors (N_d) where Fig 4 (a) – (d) represents the V_{oc} , J_{sc} , FF and η respectively of solar cell with respect to doping concentration of donors (N_d)

Figure 5

The performance of modelled solar cell with variation in effective conduction band density (N_c). Fig 5(a) – 5(d) represents the V_{oc} , J_{sc} , FF and η respectively of solar cell with respect to effective conduction band density (N_c)

Figure 6

The performance of modelled solar cell with variation in texturing angle where Fig 6 (a) – (d) represents the Voc, Jsc, FF and η respectively with respect to texturing angle.

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