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# Numerical Analysis of Metal Poly-Si Contact in TOPCon Solar Cells Through Device Simulations Using Sentaurus TCAD

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**Abstract.** Tunnel oxide passivated contact (TOPCon) is an emerging technology for highly efficient with excellent passivation photovoltaic (PV) devices. However, a standard TOPCon cell suffers from insufficient efficiency gain and recombination losses due to the presence of a direct metal-crystalline silicon contact. Therefore, bifacial configurations with advanced passivated structures have been considered in this research work. In this work, the performance of bifacial TOPCon device with double-side (DS) TOPCon structures, integrated with poly-Si, is explored and modeled using Sentaurus TCAD software. The reported study develops a framework to obtain state-of-the-art bifacial TOPCon structures with optimized input parameters and considering tunneling structures. The impact of collective front/rear $SiN_x$ layer thickness (from 50 to 100 nm) and p+ poly Si thickness (from 20 to 100 nm) on the performance of bifacial-DS TOPCon solar is studied and analyzed for optimized PV performance. This research study reveals that optimizing the p+ poly-Si thickness enhances carrier collection with minimal bulk recombination losses. The PV performance of DS structure indicates that incorporating DS carrier selective contacts increases the PV efficiency. Also, the detailed analysis of bifacial TOPCon structure reveals that suppressing the recombination by incorporating tunneling structures on both sides can be the key strategy to improve PV performance with an optimized efficiency of 26.3%. The reported study set a clear direction for higher PV performance by incorporating a tunneling approach in next-generation c-Si solar cells at low cost.

**Keywords:** Bifacial, Silicon, Simulations, Solar Cell, TOPCon

## 1. Introduction

Nowadays, poly-Si based advanced solar cells known as tunnel oxide passivated contact (TOPCon) cells have emerged as effective solutions for high photovoltaic (PV) performance [1], [2]. These structures received more consideration due to their excellent passivation performance, high stability, low recombination current density, reduced contact resistivity, and higher selectivity of charge carriers by decoupling the recombination-active areas from the Si substrate [3]. The development of high-efficiency solar cells is important to meet the rising demands for electricity globally. Thus, increasing the PV devices efficiency further lowers the levelized cost of energy (LCOE) for solar-generated power and increases energy generation [4]. In the 1980s, the concept of poly-Si passivating contacts was initially proposed, which set the stage for the advancement of passivated contact technologies [5], [6]. With a 23% efficiency in silicon PV, the TOPCon structure, which was first developed by Fraunhofer ISE in 2014, was a significant achievement [7], [8]. Afterwards, in 2017, the idea of a selective emitter was considered for TOPCon structure by Fraunhofer ISE to develop the PV technology and set a new lab-scale efficiency record of 25.7% [9]. Trina Solar developed the first 24.58% commercial TOPCon solar cell for industrial-scale usage in 2019 and made a significant advancement on a 244.62 $cm^2$ area [10]. Recently, a theoretical efficiency limit of 28.7% has been reported [11]. By using the latest laser-enhanced contact optimization (LECO) process at optimized sintering temperature of 790 °C, authors have achieved 25.98% efficient TOPCon device [12]. Wang et al. [13] obtained 25.1% efficiency using Jolywood Special Injected Metallization (JSIM) firing process which reduces the line resistance of first finger because of customised paste utilisation. Jinko et al. [14] reported 26.4% efficient n-type TOPCon having area of 334.9 $cm^2$. Whereas, However, the industrial efficiency range of TOPCon solar cells falls between 24% to 25% suggesting that TOPCon devices still have an option for further improving the conversion efficiency. These devices are unique owing to their combination of a strongly doped poly-Si layer and an ultrathin interfacial oxide ($SiO_x$) layer. Due to their rapid industry adoption and current position as the dominant technology in the market, single-side (SS) and double-side (DS) passivated contacts are the subject of the majority of device simulations [15]. The presence of poly-Si layer on the rear side of commercially manufactured TOPCon devices is limited due to parasitic absorption issues [16], [17]. However, there has been increasing interest in including the TOPCon layer on the front side of solar cells, either as a thin coating of poly-Si covering the full surface or as a layer of poly-Si that is limited to the area directly beneath the front metal contacts termed as double side (DS)-TOPCon solar cells [18]. As per industrial research, DS-TOPCon cells are considered to be appropriate as bottom cells for Si-perovskite tandem devices, which may result in higher $V_{OC}$ exceeding 730 mV [19]. Hence, DS-TOPCon devices have gained much attention due to potential for attaining >26% efficiency [20].

Previous published studies revealed that approximately 50% of recombination happens due to front side of the TOPCon structure, making it an important area for improvement. The research community has put a lot of effort into addressing FF and $V_{OC}$ losses with optimized solutions in order to enhance the PV performance of TOPCon devices. Zhou et al. [21] have reported that by reducing the front surface field recombination and contact area, an increment in PV performance has been achieved. Wang et al. [12] reported 25.97% efficient TOPCon solar cell by including the laser-enhanced contact optimization (LECO) process with low recombination current density ($J_o$). Whereas, Liu et al. [22] have achieved 25.17% conversion efficiency with optimized $p^+$ layer boron concentration of $8.68 \times 10^{18}$ atom/$cm^3$ with a depth of 0.53 µm, while the concentration in $p^{++}$ layer is $2.35 \times 10^{19}$ atom/$cm^3$ with a depth of 0.82 µm. As per the literature, it is observed that PV performance of TOPCon solar cells is highly influenced by structural parameters such as wafer thickness, half-finger pitch, and bulk lifetime of the c-Si substrate etc.

In this contribution, the performance of bifacial TOPCon solar cell with double-sided (DS) passivating contacts has been designed, studied and analyzed using Sentaurus TCAD software. The reported bifacial structure design has passivating contacts on both sides, termed as double-sided (DS) topology. The PV performance of the reported device is analyzed through PV parameters (Power conversion efficiency; PCE, open circuit voltage; $V_{OC}$, short current density, $J_{SC}$ and Fill factor; FF). The modeling results based on published experimental data provide insights into optimization pathways for high-efficiency TOPCon cells.

## 2. Simulation Framework

The device simulations for TOPCon solar cell are performed using industry-processed Sentaurus TCAD software. The cross-sectional schematic view of bifacial DS-TOPCon structures is depicted in Figure 1. Whereas, all the input parameters that are used for device simulations are tabulated in Table 1 and the models are mentioned in Table 2. All device simulations are performed under standard test conditions (STC): AM1.5G solar spectrum at 300 K [23] . Optical simulations are performed to generate the optical generation profiles using a ray tracer model before performing the electrical simulations. For designing the devices, *n-type* Si wafer (doping $5\times10^{15}$ $cm^{-3}$, resistivity: ~1 Ω-cm) is taken as the substrate (absorber) of 130 µm. The same doping can be calculated and verified through material properties from PVCDROM [24], [25]. Initially, optimized substrate thickness of 130 µm is considered to achieve the higher PV performance as predicted in the ITRPV-2024 [15]. For TOPCon devices, the tunnel oxide layer sandwiched between poly-Si and Si-substrate plays a vital role in passivation and charge carrier transport. The optimized thickness of $SiO_x$/Poly-Si on rear side of the device is 1.2 nm/120 nm for bifacial DS-TOPCon is considered. Here, half-finger width solar cells are investigated using TCAD simulations. Further, silicon nitride ($SiN_x$) is employed on front side owing to its dual role as antireflection coating and passivation. To fully utilize the bifaciality concept, a dielectric stack (oxide/poly-Si/$SiN_x$) is incorporated on rear side to reabsorb the reflected light. Different models, such as Richter for auger recombination [26], Klaassen model for mobility [27] and Schenk bandgap narrowing model [28] for heavily doped areas. Also, the non-local carrier tunneling model [29] accounts for the tunneling of charge carriers.

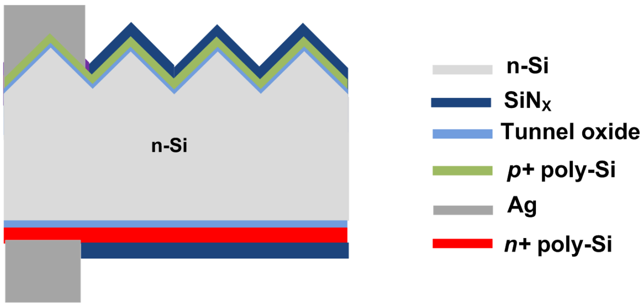



***Figure 1.*** *The schematic view of bifacial double-side (DS) TOPCon solar cells (not to scale)*

***Table 1.*** *Input and modeling parameters used in TCAD device simulations.*

| Parameter Description | n-TOPCon (DS; Bifacial) |
|---|---|
| Bulk thickness (µm) | 130 [30] |
| Bulk lifetime (ms) | 10 [18, 31] |
| Bulk resistivity (Ω-cm) | ~2 [22, 32] |
| Substrate doping ($cm^{-3}$) | $5\times10^{15}$ |
| Front $p^+$ poly-Si Doping ($cm^{-3}$) | $1\times10^{20}$ |
| Thickness of front tunnel oxide (nm) | 1.2 |
| Calibrated front $p^+$ poly-Si thickness (nm) | 150 nm [3] |
| Front $p^+$ poly-Si thickness after calibration (nm) | Variable |
| Front poly-Si/SiOx interface SRV (cm/s) | 0.9 |
| Front poly-Si defect density ($cm^{-3}$) | $10^{17}$ |
| Rear $n^+$ poly-Si thickness (nm) | 120 [33] |
| Rear poly-Si/SiOx interface SRV (cm/s) | 1 |
| Rear poly-Si defect density ($cm^{-3}$) | $10^{17}$ |
| Rear $n^+$ poly-Si Doping ($cm^{-3}$) | $2\times10^{20}$ [33] |
| Thickness of rear tunnel oxide (nm) | 1.2 [22] |
| Silicon nitride thickness on front/rear (nm) | Variable |

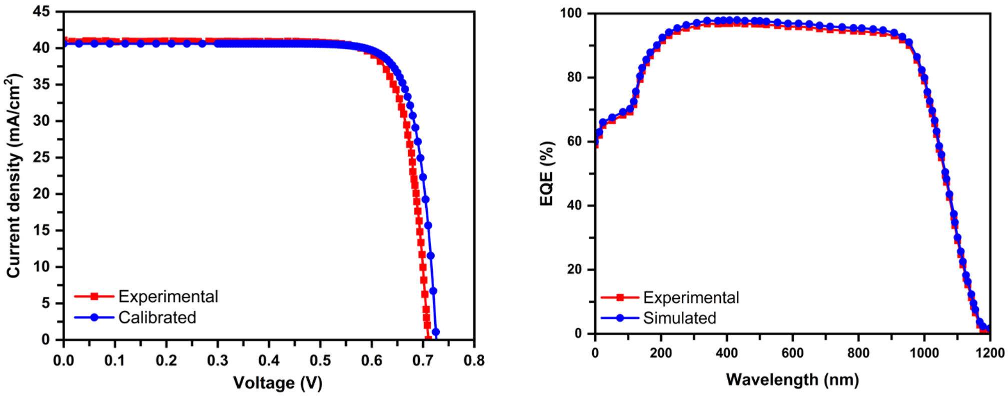
***Table 2.*** *Summary of models used for device simulations.*

| | |
|---|---|
| Non-local carrier tunneling model | Stodolny [29] |
| Mobility | Klaassen [27] |
| Auger recombination (300 K) | Richter [26] |
| Bandgap narrowing | Schenk [28] |
| Light Source and Temperature | AM15.G intensity 1kW/$m^2$ [34] at 300K |
| Effective tunneling mass | $m_{te} = 0.40m_o$, $m_{th} = 0.32m_o$ [35], [36] |

# 3. Results and discussion

Initially, the calibration of the bifacial n-TOPCon device (single side TOPCon structure) has been performed as per experimental results reported in literature [3], along with tabulated models in Table 1. A calibrated and experimental illuminated current-density (JV) and external quantum efficiency (EQE) curves have been obtained, as shown in Fig. 2 (a-b). Authors have reported 23.01% efficiency [3] through experimental study, but by considering the same reported experimental input parameters, we have obtained 23.70% efficiency using TCAD models. The close alignment of PV performance via a calibration study shows the accuracy of physical models and input parameters. As per Fig. 2, simulated $V_{oc}$ is slightly higher than experimental because the model was first calibrated using a bulk lifetime of 8 ms, following Ref. [3], which reproduced the experimental device performance with only a small deviation. For consistency, a bulk lifetime of 10 ms was then used in all subsequent simulations to represent slightly improved wafer quality and to standardize the analysis across all parametric studies.

Here, the performance of bifacial DS-TOPCon is investigated by doing the parametric optimization. It is noteworthy that n+ passivating contacts offer low contact resistivity to electrons while blocking the path of holes. Similarly, p+ passivating contact enables hole tunnelling and acts as a barrier for electrons. In this manner, DS-TOPCon structures avoid the charge carrier recombination by facilitating the tunnelling of electrons from rear side and holes from front side. Thus, this reported bifacial DS-TOPCon enhances the device performance with double-side TOPCon concept. Along with this, as PV industry is rapidly moving towards ultra-thin wafers owing to higher flexibility, lower material usage cost and less energy consumption during wafer production, it becomes important to look into how PV performance is affected with variations in device parameters. So, after performing the calibration for bifacial SS-TOPCon device (as depicted in Figure 2), we made the changes in structure to make it bifacial DS-TOPCon by following the same models and input parameters as tabulated in Table 1 while keeping the $p^+$ poly-Si thickness at 35 nm.




(a) (b)

***Figure 2.*** *(a) Illuminated JV curve and (b) EQE of calibrated bifacial n-TOPCon solar cell; calibration is done with experimental data [3]*

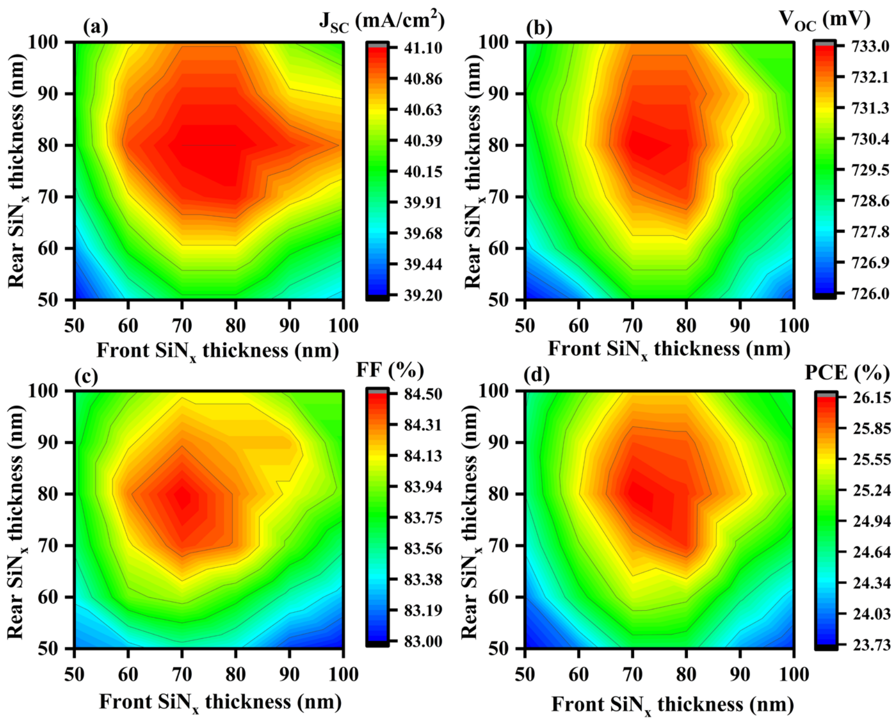



***Figure 3.*** *The collective impact of front and rear $SiN_X$ thickness on PV parameters (a) $J_{SC}$, (b) $V_{OC}$, (c) FF and (d) PCE*

The influence of collective front and rear $SiN_x$ thickness (from 50 to 100 nm) has been studied and analyzed as given in Figure 3 (a-d). As $SiN_x$ is used for ARC and passivation purposes, its optimal thickness significantly influences the PV performance. To visualize the $SiN_x$ thickness, collectively variations for both front and rear have been performed. From the obtained results, it has been observed that maximum light trapping and higher PV performance (PCE) are achieved when thicknesses are in the range of 70-80 nm for both front and rear $SiN_x$ thickness.

If the thickness is too thin, then PCE will reduce due to a reduction in $J_{SC,}$ having higher optical losses with minimal variation in $V_{OC}$ and FF. If its thickness is too thick, then it could hinder the penetration of silver paste during screen printing and result in higher contact resistance. Through these collective analyses, the optimized thickness for both and rear $SiN_X$ is 70 nm/70 nm, which provides better PV performance (26.15%).

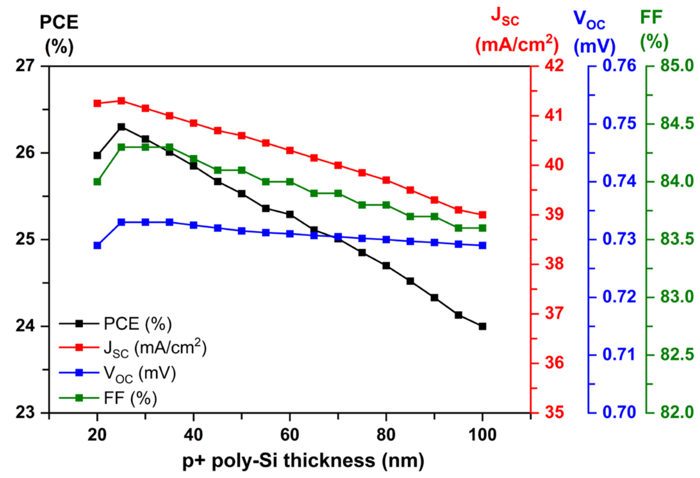



***Figure 4.*** *The influence of p⁺ poly-Si thickness on PV parameters (a) $J_{SC}$, (b) $V_{OC}$, (c) FF and (d) PCE*

After optimizing the $SiN_X$ thicknesses, the influence of front $p^+$ poly-Si thickness from 20 to 100 nm has been studied, as it also affects thermal stability. If the thickness of p+ poly-Si is too thick, then it will result in higher recombination due to oxide disruption, boron penetration at high firing temperatures and higher parasitic absorption losses [37, 38]. From the results, it has been noticed that $J_{SC}$ decreases at higher thickness because of parasitic absorption and the highest $V_{oc}$ is obtained when the thickness of the poly-Si layer is between 20-30 nm. While such thicknesses have been experimented with earlier with some success, firing stability and metal penetration through the poly-Si layer remain areas of concern [39]. Similarly, FF decreases due to higher series resistance. The impact of all three parameters is reflected in conversion efficiency (Fig. 4(d)). It can be seen that the optimized p+ poly-Si thickness ~25 nm [40] which results in highest efficiency (26.3%).

## 4. Conclusion

In this study, bifacial TOPCon structure with double-sided passivating contacts has been designed and simulated through the Sentaurus TCAD tool. The performance of bifacial-DS TOPCon is studied and analyzed by varying the input parameters. From the results, it is found that optimization of input parameters plays an important role in maximizing the PV performance. It has also been observed that the incorporation of passivating contacts on both sides results in better performance with minimum recombination losses, better passivation and improved carrier collection efficiency. The optimized PV performance of bifacial-DS TOPCon is 26.3% at 70 nm/70 nm of $SiN_x$ thickness on both front and rear sides by including 130 µm optimized substrate thickness. The reported research work confirms the viability of the device structure through TCAD simulations. The concept of laser-enhanced contact optimization (LECO) process could be included in the proposed devices for further enhancement of PV performance in the future.

## Data availability statement

The data that support the findings of this study are available upon reasonable request from the first author.

## Author contributions

Savita Kashyap: Conceptualization, Methodology, Software, Data Curation, Formal Analysis, Investigation, Visualization, Writing – Original Draft

Shiladitya Acharyya: Software, Investigation, Technical Support (Sentaurus TCAD)

Durga Prasad Khatri: Software, Investigation, Technical Support (Gridler Metallization Analysis)

Pradeep Padhamnath: Formal analysis, Methodology, Conceptualization, Writing – Review & Editing

Anil Kottantharayil: Funding Acquisition, Supervision, Validation, Formal Analysis, Writing – Review & Editing

## Competing interests

The authors declare that they have no competing interests.

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