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Numerical simulations of IBC solar cells based on poly-Si carrier-selective passivating contacts

Paul Procel, Guangtao Yang, Olindo Isabella, Miro Zeman

Abstract—This work presents an analysis of physical mechanisms related to operation and optimization of IBC polysilicon based devices. Concepts of carrier selectivity and tunneling are used to identify parameters that impact on the fill factor. Then, based on TCAD numerical simulations, we describe the device performance in terms of transport and passivation. A validation of the model is performed by matching measured and simulated R, T and EQE spectra and electrical parameters. As result of such process, the opto-electrical losses of the reference device are identified. Then, we execute a study of the impact of process parameters on the performance of the IBC device under analysis. Assuming uniform SiO$_2$ layer, simulation results reveal that both n-type and p-type poly-Si contacts can be theoretically perfect (i.e. approx. lossless), if assuming no interface recombination but considering tunneling of both carrier types. In other words, there exists an optimum oxide thickness (1 nm) for which majority carriers tunneling works already very well, and minority tunneling is still low enough to not result in significant recombination. Moreover, SiO$_2$ thickness up to maximum 1.6 nm is crucial to achieve high efficiency. Regarding rear geometry analysis, the efficiency curve as function of emitter width peaks at 70% pitch coverage. Further, it is shown that diffused dopants inside c-Si make the device resilient to passivation quality. Finally, the calibrated model is used to perform an optimization study aiming at calculating the performance limit. The estimated performance limit is 27.3% for a 100-µm thick bulk, 20-nm thick polysilicon layers, silver as rear contact and double ARC.

I. INTRODUCTION

Crystalline Silicon (c-Si) solar cells are leading the actual photovoltaic market due to abundance of raw material, stability, technological development, conversion efficiency and cost-effectiveness [1]. Simultaneously, the photovoltaic (PV) market aims at reducing costs of generated electrical power by increasing solar cells efficiency and minimizing production cost. To achieve this objective, research and development groups devoted several works on novel concepts to reduce device recombination losses and on advanced solar cell architectures [2]. Concerning solar cell architectures, interdigitated back contact (IBC) concept stands as the main option to demonstrate remarkable efficiencies [3]–[8] owing to the absence of front shading contact. To increase the conversion efficiency of solar cells, it is crucial to reduce the recombination losses that are typically related to highly defective metal/semiconductor interfaces in conventional homo-junction devices. One approach to quench such recombination losses consists in reducing metal/c-Si interface using point contacts. However, this approach demands additional lithography steps with still limited open-circuit voltage (V$_{oc}$) [9]–[11] (below 700 mV). On the other hand, passivating carrier-selective contacts (CSCs) effectively reduce such recombination losses, demonstrating high V$_{oc}$ well above 715 mV for high [12]–[14] and low temperature processes [6], [8], [15]–[17]. High-thermal budget CSCs commonly deploy a thin SiO$_2$ passivating layer beneath highly-doped poly-silicon (alloys). This approach is of particular interest owing to its compatibility with industrial thermal budgets. Moreover, recent results report outstanding V$_{oc}$ values well above 700 mV [14], [18]–[25], anticipating conversion efficiency above 26% [3] when combining CSCs with IBC solar cell architecture. Like silicon heterojunction contacts based on hydrogenated amorphous silicon, the core of such high efficiency devices stands on transport mechanisms. Several studies have been reported to explain the inner physics of poly-silicon based CSCs. Accordingly, two different approaches have been proposed to describe transport though the thin oxide layer: (i) carrier transport via pin-hole in oxide layer [26], [27], and (ii) tunneling of carriers trough ultra-thin oxide layers [28], [29]. In the first case, pin-holes are formed by increasing the annealing temperature above 1000 °C in oxide layers above 2 nm [20]. In the second case, the transport of carriers is described by tunneling through a potential energy barrier built by an oxide layer around 1.5-nm thick [22], [30]–[33], implying process temperatures lower than 950 °C. It is worth noting that several studies within state-of-art CMOS devices [34]–[40] confirm that leakage currents though thin dielectrics are based on tunneling. In such a context, theoretical works describing transport mechanisms have been carried out to explain the potential of CSCs based on oxide as passivating layer [28], [41] for front and rear contact structures.

Here, based on an advanced two-dimensional opto-electrical model, we investigate the mechanisms leading to main losses in poly-Si based IBC reference solar cell [22]. After, we identify the main competitive physical mechanisms that are related to process fabrication and enable high fill factor (FF)
II. CONTACT SELECTIVITY AND TRANSPORT

A. Contact Selectivity

Considering the definition of contact selectivity (S) proposed in [49] at the latest portion of c-Si, beneath the tunneling oxide interface, we have:

$$S_n = \frac{n \cdot \mu_e}{p \cdot \mu_h} ; \quad S_p = \frac{p \cdot \mu_h}{n \cdot \mu_e} \quad (1)$$

where \( n \) and \( p \) are electrons and holes concentration, and \( \mu_e \) and \( \mu_h \) are electron and hole mobility. As in c-Si \( \mu_e \) and \( \mu_p \) are in the same order of magnitude, the fundamental of high selectivity stands on the asymmetric carrier concentrations at the interface [49]. Accordingly, the contact selectivity is maximized by increasing the carrier concentration of one type of carriers and dually decreasing the concentration of the other.

Since selectivity and transport of poly-Si based CSC are symmetrical for collecting electrons or holes (see Figure 1), we describe physical mechanisms related to electrons in the conduction band as reference. Such an assumption is here valid as poly-Si features a band gap close to that of c-Si; then, similar phenomena are expected for holes in the valence band. In general, carrier concentrations at c-Si / SiO\(_2\) interface are so defined:

$$n = \Delta n + N_D = N_C \cdot e^{\left(\frac{E_{f,cSi} - E_{f,cSi}^\text{fn}}{kT}\right)} = N_C \cdot e^{\left(\frac{\Delta E_e}{kT}\right)} \quad (2)$$

where \( N_C \) is the density of states in the conduction band for electrons, \( E_{f,cSi}^\text{fn} \) stands for Quasi-Fermi energy level of electrons at c-Si / SiO\(_2\) interface, \( E_{f,cSi} \) is the conduction band energy, \( N_D \) is donor density and \( \Delta n \) is the free carrier injection density. Thus, for n-type contact at the c-Si / SiO\(_2\) interface, \( n \) is maximized when \( \Delta E_e = E_{f,cSi} - E_{f,cSi}^\text{fn} \) is a negative number, meaning that \( E_{f,cSi} < E_{f,e,cSi} \) while, for p-type contact and at the c-Si / SiO\(_2\) interface, \( p \) is maximized when \( \Delta E_h = E_{f,h,cSi} - E_{f,h,cSi}^\text{fn} \) is negative, in other words \( E_{f,v,cSi} > E_{f,v,cSi}^\text{fn} \). This can be attained by maximizing the band bending in c-Si leveraging on the built-in voltage (\( V_{bi} \)) [50]. In case of silicon heterojunction (SJH), to induce a strong c-Si band bending, contact material fabrication process allows flexibility to set the proper Fermi energy for maximized \( V_{bi} \) at low temperature [50]. If contact material properties do not allow a strong band bending (i.e. poly-Si alloys), \( n \) and \( p \) can be also maximized with the support of active dopants diffused inside c-Si as result of dopants activation temperature [51]. Importantly, according to equations (2), \( \Delta E_e \) and \( \Delta E_h \) are also minimized if doping peak concentration at c-Si / SiO\(_2\) interface is higher than \( N_C \) (3.2x10\(^{19}\) cm\(^{-3}\)) for n-type contact and higher than \( N_V \) (1.8x10\(^{19}\) cm\(^{-3}\)) for p-type contact, thus maximizing contact selectivity.

B. Tunnelling

In CSCs-IBC solar cells, the collection of carriers involves transport through two hetero-interfaces. Poly-Si CSC interfaces consist of (i) c-Si passivated by thin SiO\(_2\) layer subsequently (ii) covered by highly doped poly-Si layer. Such structures exhibit peculiar discontinuities in the band diagram,
as Figure 1a and 1b show. Assuming uniform (i.e. no pin-holes) SiO$_2$ layer, carrier collection is described by tunnelling transport mechanisms. These mechanisms describe the transport of carriers with enough energy to cross through a potential energy barrier. The energy of carriers, the occupied and free states in both sides of the barrier and the energy barrier are therefore crucial parameters. As described in Leong et al. [45], the tunnelling for transport of electrons and holes is therefore related to the local generation rate $G$ as follows:

$$G_e = \frac{A \cdot T}{k} \cdot \xi \cdot \Gamma_e (r_{ox}) \cdot \ln \left( \frac{1 + \exp \left( \frac{-\Delta E_e}{kT} \right)}{1 + \exp \left( \frac{-E_{c,csi} - E_{f,e,n}}{kT} \right)} \right)$$  \hspace{1cm} (3)$$

where $A$ stands for Richardson constant, $T$ is temperature, $k$ is the Boltzmann constant, $\xi$ is the electrical field, $\Gamma_e (r_{ox})$ is the tunnelling probability in SiO$_2$ layer, $\Delta E_e$ is the energy of collecting carriers at c-Si/SiO$_2$ interface with respect to Fermi energy ($E_{f,c,csi} - E_{f,e}$) of electrons in the conduction band and $E_{f,e}$ is the Quasi Fermi-level of electrons at each side of energy barrier, either c-Si / SiO$_2$ (c-Si) or doped poly-silicon / SiO$_2$. The subscripts $n$ indicates n-type contact. The term inside the logarithm correlates the density of filled states and free states at each side of energy barrier [34]. As the density of filled states at the c-Si / SiO$_2$ interface is associated to equations (2), maximizing collecting carrier density improves the transport of carriers. In case of poly-Si CSCs, such an effect is achieved thanks to active dopants inside c-Si. It is worth noting that transport of carriers in poly-Si CSCs is deployed in the conduction (valence) band for n-type contact (p-type contact) featuring the so-called direct tunnelling. The tunnelling probability $\Gamma_e (r_{ox})$ is calculated following Wentzel-Kramers-Brillouin (WKB) approximation:

$$\Gamma_e (r_{ox}) = \exp \left[ -\frac{2}{\hbar} \int_0^{r_{ox}} \sqrt{2m_e \left( E_{f,e,n} - E_{c,csi} - q\psi_e (r) \right)} \, dr \right]$$  \hspace{1cm} (4)$$

where $\hbar$ is the reduced Planck constant and $\psi_e (r)$ is the electrostatic potential in terms of potential barrier profile along the position $r$ for electrons, $m_e$ are the tunnelling masses of electrons and holes, respectively. TCAD Sentaurus considers a complex state-of-art model detailed in [45], [52] to describe transport through interfacial barriers by tunnelling. However, the purpose of this work is to only identify parameters affecting the collection of carriers through tunnelling oxide in poly-Si based CSCs. For this reason, we assume an exceptionally simplified thin oxide energy barrier as a rectangular barrier defined by a potential energy ($E_R$) and oxide thickness ($r_{ox}$) (see Figure 1). With such an assumption, we account similar bandgap for poly-Si and c-Si. Then, equations 4 is simplified to:

$$\Gamma_e (r_{ox}) = \exp \left[ -\frac{2r_{ox}}{\hbar} \sqrt{2m_e \left( E_{be} - E_{c,csi} \right)} \right]$$  \hspace{1cm} (5)$$

Interestingly, $r_{ox}$, $m_e$, $E_{be}$ and $E_{bh}$ have an exponential impact on $\Gamma (r_{ox})$, which contribute to define the current behavior [34], [45], [52] through $G_e$ and $G_h$. From this approach, $m_e$, $E_{be}$ and $E_{bh}$ are parameters inherent to the dielectric material used as tunnelling oxide (uniform SiO$_2$), but $r_{ox}$ is related to device process.

## III. Simulation Methodology

Figure 2 shows the two-dimensional (2-D) cross-section of the poly-Si IBC solar cell symmetry element used to perform opto-electrical simulations. The model has been developed based on a reference IBC solar cell featuring a 280-µm thick, 5 Ω-cm resistivity FZ c-Si n-type wafer and a 650-µm wide pitch [22]. Consistent with processed device, the front interface is texturized by random pyramids and covered by a thermal SiO$_2$/PECVD Si$_3$N$_x$ anti-reflective coating (ARC).

Similar to [53], the front texturing was modeled by a sequence of triangles with a fixed base angle of 54.7° related to the wet-etching process, featuring a maximum height of 5.6 µm. The rear hole- and electron-selective contact interfaces are planar and disconnected by a 1-µm large curved gap that results from the self-aligned process [22]. To passivate the rear side of c-Si absorber bulk, a 1.5-nm thick tunneling SiO$_2$ layer is formed by means of Nitric Acid Oxidation of Silicon (NAOS) [54]. The front surface field (FSF) is formed by phosphorus implantation. The n-type contact and the p-type contact are formed by 250-nm thick LPCVD poly-Si subsequently implanted with P and B, respectively [22], then annealed at 950 °C and finally hydrogenated. Doping profiles were extracted from electrochemical capacitance (ECV) measurements to obtain the doping profiles of the reference IBC solar cell [22].

### A. Models and Parameters

The device model has been developed on finite element
numerical simulator TCAD Sentaurus [52], according to the geometrical and physical parameters of the reference poly-Si IBC cell. The simulation approach is similar to the one described in [53]. Thus, the optical simulation is performed by using the internal ray-tracing model and free-carrier absorption (FCA) has been modeled assuming the doping concentration as carrier concentration [55]. The electrical simulation is based on a drift-diffusion model, using state-of-art models [56], [57] for AM1.5G illumination [58]. It should be noted that optical and electrical simulation share the same simulation domain, then the 2-D optical generation rate obtained from the optical simulation is directly set into the electrical simulation stage [53].

A summary of parameters of the processed device used in this work is presented in Table I.

<table>
<thead>
<tr>
<th>Parameter/Model</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk resistivity</td>
<td>5 Ωcm</td>
</tr>
<tr>
<td>Substrate thickness</td>
<td>280 μm</td>
</tr>
<tr>
<td>Pitch</td>
<td>650 μm</td>
</tr>
<tr>
<td>Poly-Si thickness</td>
<td>250 nm [22]</td>
</tr>
<tr>
<td>SiO₂ thickness</td>
<td>1.5 nm [22]</td>
</tr>
<tr>
<td>FSF doping peak</td>
<td>1x10¹⁰ cm⁻³ [66]</td>
</tr>
<tr>
<td>n-contact doping</td>
<td>Doping profile (1x10¹⁰ cm⁻³ [22])</td>
</tr>
<tr>
<td>p-contact doping</td>
<td>Doping profile (1x10¹⁰ cm⁻³ [22])</td>
</tr>
<tr>
<td>Contact Resistance</td>
<td>0.3 mΩ²cm⁻²</td>
</tr>
<tr>
<td>Finger and bus bar resistance</td>
<td>Distributed model: 1.6 Ω²cm</td>
</tr>
<tr>
<td>Tunneling Model</td>
<td>Non-local Tunneling model [52]</td>
</tr>
<tr>
<td>Effective tunneling masses for holes and electrons</td>
<td>m_n=0.4 m_e; m_n=0.32 m_e [34]</td>
</tr>
</tbody>
</table>

m_e is the electron rest mass. Doping profiles of n-type and p-type contacts are extended to c-Si according to [22].

The calibration of Shockley-Read-Hall (SRH) bulk and surface recombination parameters (bulk lifetime, τ_bulk, and surface recombination velocity, SRV) were extracted from the validation process in which we compared simulated and measured current density - voltage (J-V) and external quantum efficiency (EQE) curves. Since our reference poly-Si IBC solar cell was processed at temperatures around 950 °C, we assume that collection of carriers in poly-Si CSCCs is characterized by tunneling mechanisms [28], [29]. These were modelled according to the non-local model implemented in TCAD Sentaurus [52].

B. Validation

The set-up opto-electrical platform was used to simulate, reflectance (R), EQE, transmittance (T) and J-V curves related to the real device. Accordingly, the device model was calibrated in terms of SRH parameters, which are not material dependent [53]. Figure 3 shows the comparison between measured and simulated R, T, EQE, IQE spectra. Similarly, Figure 4 depicts the comparison between measured and simulated J-V curves. In general, we observed a good agreement between simulated and measured data in both spectral behavior and electrical characteristics, confirming that our simulation platform describes accurately the physical mechanisms occurring in the reference device, including tunneling models.

IV. SIMULATION RESULTS

A. Optical and Electrical Loss Analysis

Resulting from the validation, we identified and extracted the main losses affecting the conversion efficiency of the reference device. These mechanisms were spectrally analyzed in the
wavelength range between 300 nm and 1200 nm. We estimated R, T, free carrier absorption (FCA) and parasitic absorption in front SiN, layer and rear metallic contacts. Then, recombination losses were evaluated. Figure 5 shows the quantification of optical and electrical losses for the reference poly-Si IBC solar cell. Considering ASTM 1.5G spectrum, every loss contribution was estimated in terms of implied current density (mA/cm²). Main losses were due to recombination (2.41 mA/cm²), reflectance (2.05 mA/cm²) and FCA (1.33 mA/cm²) (see Figure 5a). Looking into the recombination losses, they were mainly localized at front interface (41%) and c-Si bulk (51%) (see Figure 5b).

Table II summarizes the recombination parameters, allowing for model calibration. At n- and p-contact interface, such values match with those calculated from symmetrical samples [22]. However, it was revealed that main losses occur at the textured front interface (SRV F = 5000 cm/s). Considering the relatively low J sc,FSC = 31 fA/cm² reported in [22] for a symmetrical test sample, this effect is ascribed to the introduction of interface defects during the patterning process. Improved the cleanliness of such process and keep constant the others according to Table I and Table II. Additionally, to evaluate the potential performance of the solar cell, simulation results include two scenarios: (i) reference device parameters, and (ii) almost ideal parameters but still realistic state-of-art technology (see Table II). Note that transport effects are quantified in terms of FF and recombination effects are apparent in terms of V oc and J sc values.

B. Transport

1) Tunneling Oxide thickness

As mentioned in Section II, SiO₂ thickness r ox exponentially influences tunneling transport of carriers in terms of tunneling probability Γ in equations (4), (5), (8) and (9). Such an effect is apparent in Figure 6, depicting the strong degradation of FF and η when r ox increases. A sharp efficiency decrease is observed for oxide thickness values larger than 1.6 nm. A reduction of r ox from 1.6 to 1.5 nm improves efficiency by 2.5% abs, while a further decrease of r ox from 1.5 to 1 nm enhances the efficiency by another 0.7% abs. As mentioned in Section II-B, the generation rate associated to tunneling (equation 3) depends on the potential barrier size, the filled states and the available states in both sides of such a barrier. The variation of tunneling oxide thickness affects not only the collection of collecting carriers but also the transport of non-collecting carriers. Therefore, Figure 6 reports that conversion efficiency and FF are maximized for 1 nm r ox. The decrease in efficiency for r ox < 1 nm is explained in terms of less effective barrier for non-collecting carriers. Indeed, reducing r ox, contact
passivation becomes less effective and carrier collection tends to be similar to homo-junction devices with lower $V_{oc}$. On the other hand, the decrease in efficiency for $r_{ox} > 1$ nm is explained by the reduced transport of collecting carriers in terms of lower tunneling probability. It is worth noting that for semiconductor applications $r_{ox}$ thicknesses within 0.9 nm and 1.5 nm thickness are attainable depending on oxidation method [59], [60].

In general, higher $\eta$ are achieved for 1-nm thick $r_{ox}$ due to the improvement of transport of collecting carriers through the energy barrier of the layer, keeping an effective barrier for transport of non-collecting carriers. This effect emphasizes the sensitivity of solar cell transport to SiO$_2$ thickness, becoming critical at 1.6 nm. In particular, a 1-nm thick $r_{ox}$ maximizes the conversion efficiency to 22.1%, assuming extracted recombination parameters, and to 25.9% considering ideal parameters case.

2) Rear Geometry
Typically IBC solar cells deal with lateral transport for collecting carriers [61]–[63] in terms of rear side geometry. Thus, to evaluate the impact of lateral transport on our poly-Si IBC device, we performed a set of simulations varying the p-type contact width, keeping constant the pitch and the connecting gap. In other words, smaller p-type contact fingers (emitter) entail a wider n-type contact fingers (back surface field) and vice versa. Simulations were run for a range of p-type contact (n-type contact) width from 150 to 440 $\mu$m (from 500 to 210 $\mu$m), assuming constant all the other parameters. Accordingly, the equivalent so-called p-type contact coverage is changed from 20% to 84%. Figure 7 shows $J_{sc}$, $V_{oc}$, FF and $\eta$ as...
a function of p-type contact width for both the reference and the ideal poly-Si IBC devices. In general, the so-called electrical shadowing effect for homo-junction IBC solar cells [62], [64] is almost negligible as $J_{sc}$ and $V_{oc}$ trends demonstrate in Figure 7a and 7b in case of the ideal device. Indeed, differently than IBC homo-junction solar cells, IBCs with CSC feature similar passivation for both contacts, then $J_{sc}$ and $V_{oc}$ are almost independent from rear side geometry. However, it is worth noting that in case of the reference device, recombination effect becomes apparent as $J_{sc}$ thanks to the dominant front recombination calculated for reference device (see Table II). Interestingly, a bell-shaped curve is observed in FF case featuring a clear maximum value at 78.4% (82.4%) for a p-type contact width of 452 μm (or 69% pitch coverage) for reference (ideal) device. Such a trend reveals transport issues occurring in thin oxide layer as result of crowded tunneling current in case of electrons for smaller n-type contact width and crowded tunneling of holes in case of small p-type contact. Hence, the maximum FF results from the trade-off between tunneling currents of electrons and holes in terms of optimal p-type contact coverage. Looking into Figure 7c and 7d, the trend of FF dictates that of $\eta$, which tops at 21.5% (25.2%) for p-type contact width value 452 μm (70% of p-contact coverage in case of both reference and ideal devices). Such a trend is reported in detail in Figure 7e) for FF evaluated for different pitch values and p-contact over pitch coverage. In fact, the FF is optimal for p-contact over pitch coverage of 70%. Similar to c-Si IBC homo-junction and heterojunction solar cells [50], [53], [62], [63], small pitch values increase FF.

C. Passivation quality

In this section, the effect of passivation quality on solar cell performance is investigated. To do so, we evaluated $V_{oc}$ and $\eta$ as function of SRV at p-type contact (SRV$_p$), n-type contact (SRV$_n$) and front (SRV$_F$). It is worth noting that SRV is related to defects at c-Si interface and can be reduced depending on interface treatment to values below 1 cm/s [65]. In each case we varied the SRV in the range between 0.1 cm/s and $1 \times 10^6$ cm/s (see Figure 8). In case of n-type and p-type contact interfaces (see Figure 8 left and center), a similar behavior is observed. The $V_{oc}$ and $\eta$ of the reference (ideal) device are almost constant close to maximum values at 690 (732) mV and 21.4% (25.15%) for SRV values lower than $1 \times 10^5$ cm/s. However, for SRV values larger than $1 \times 10^5$ cm/s, $V_{oc}$ and $\eta$ strongly decrease. This effect is ascribed to the doping profile that extends inside c-Si [22], thus inducing an electrical field passivation [62] that is effective for SRV values up to $1 \times 10^5$ cm/s. Similarly, in case of textured front c-Si interface, the reference device features an implanted doping profile which sets up a high-low homojunction. This induces an electric field passivation which keeps $V_{oc}$ and $\eta$ from massively decreasing for SRV$_F$ values up to $1 \times 10^5$ cm/s [66]. For SRV$_F$ values beyond such a threshold, $V_{oc}$ and $\eta$ strongly decrease. Such a trend is different in case of the ideal device. In fact, in absence of FSF, $V_{oc}$ and $\eta$ strongly depend on SRV$_F$ [53], allowing high performance only for SRV$_F$ value in the range of $1 \text{ cm/s}$. After this sensitivity analysis, the estimated maximum conversion efficiency is limited to 22.38% for the reference device while it is 25.2% for the ideal device with no- FSF. This difference is mainly caused by the presence of doped FSF in the reference IBC device, that increases intrinsic recombination as a drawback if SRV$_F$ is lower than 10 cm/s (see Figure 8 c).

D. Performance limit

In this section, we performed an optimization study of poly-Si based IBC solar cell. Accordingly, we considered the parameters of the ideal device (Table II) featuring $r_{ox} = 1$ nm.
In this way we reduce the potential barrier and therefore improve the transport of carriers through the SiO₂ layer. With this assumption, η = 25.9% (see Figure 6) was calculated. However, the in-diffused doping profile exceeds the doping peak value that maximizes carrier concentration at interface as discussed on Section II. Indeed, measured doping peak concentration is 1x10²⁰ cm⁻³ [22] while required values are 3.2x10¹⁹ cm⁻³ for donors (n-type contact) and 1.8x10¹⁵ cm⁻³ for acceptors (p-type contact). In this condition, both selectivity and Auger recombination are enhanced, therefore a precise doping profile has to be enforced. In this respect, a shallow Gaussian doping profile with 50-nm deep junction and doping peak 2x10¹⁰ cm⁻³ was assumed as optimal, resulting in η = 26.3% (Optimized design #1 in Table III).

This device is limited by intrinsic recombination in the absorber bulk. To reduce intrinsic recombination, two alternatives are possible: increase bulk resistivity (reduce doping) and/or reduce bulk thickness. To keep the same bulk resistivity with respect to the reference device, we analyzed the impact of the thickness of the absorber bulk on η, J_{sc}, and V_{oc} for both Al and Ag as rear contact materials. Looking at the top panel of Figure 9, J_{sc} increases as the bulk thickness increases while V_{oc} decreases. When the bulk thickness increases, the enhancement in J_{sc} is attributed to the rise of absorbed photons while the V_{oc} degradation is due to the increase of intrinsic recombination. While the trend of V_{oc} is not affected by different back reflector, the trend of J_{sc} in case of Ag contact is sensibly higher than the counterpart based on Al. Thus, the V_{oc} contribution dominates the trend of conversion efficiency, but the choice of the rear contact material sets the absolute η values. In our study we did not simulate solar cells based on wafers thinner than 100 μm for two main reasons. First, our optical simulation framework might require additional calibration due to the multiple reflection correction reported in [53]. Second, pursuing high efficiency for wafers thinner than 100 μm is currently not industrially relevant [1] and might negatively affect the FF of manufactured devices owing to mechanical stress [8]. Thus, we considered that 100 μm is the bulk thickness that maximizes the efficiency (Optimized design #2 in Table III), exhibiting V_{oc} = 754 mV. Such V_{oc} value is around 7 mV lower than c-Si V_{oc} limit [67] due to intrinsic recombination associated to doping on bulk and buried doping profile at contact interfaces. Besides, as anticipated, the effect of switching the rear reflector from Al to Ag increases the J_{sc} value by 0.3 mA/cm² and η by 0.25%, leading to η = 26.9% (Optimized design #3 in Table III).

To further improve the conversion efficiency aiming at reducing FCA losses, we carried out a set of simulations to optimize the poly-Si thickness (r_{poly}) and metal contact coverage. The optimization process was deployed according to [53]. In general, by decreasing r_{poly}, J_{sc} is improved due to FCA losses reduction, but the lateral transport losses in the poly-Si increase. However, lateral transport in poly-Si depends also on the contact coverage that it is linked to metal parasitic absorption. In fact, within this optimization process, three competitive mechanisms are identified. The first is that FCA decreases by decreasing poly-Si thickness. The second is that lateral transport loss decreases by increasing metal contact. The third is that metal parasitic absorption increases by increasing metal contact. The optimization process resulted in ΔJ_{sc} = +0.25 mA/cm² and η = 27.1% for a 20-nm thick poly-Si thickness, and 80% contact coverage (Optimized design #4 in Table III). We note that in case of using oxide thickness thicker than 1 nm and up to 1.6 nm, optimized J_{sc} and V_{oc} values remain, but FF changes as reported in Figure 6, since the performance of the device becomes limited by transport through tunneling oxide. At this point, optical losses can be potentially reduced by applying a more advanced double anti-reflective coating (ARC) [68]. Deploying an additional 100-nm thick MgF₂ layer [69] on the standard SiNₓ, we improved the J_{sc} of our simulated poly-Si IBC device by 0.23 mA/cm². The optimized design #5 in Table III summarizes the best external parameters found in this work: J_{sc} = 41.7 mA/cm², V_{oc} = 754 mV, FF = 86.7% and η = 27.3%. Interestingly, similar values are calculated for optimized IBC solar cells with silicon heterojunction scheme [50], thus revealing similar potential
performance for both type of CSCs. After this optimization process, we note a clear reduction of recombination losses that improves both $V_{oc}$ and $J_{sc}$. On the other hand, pure optical losses (R+T and $Abs_{parasitic}$) are essentially unaltered even for the optimized 100-μm thick bulk, as Figure 10 illustrates. In fact, if the dual ARC quenches primary reflectance, the deployment of Ag rear reflector, together with thinner bulk, increases the rear reflectance, augmenting the chance for long wavelength light to escape the device. At the same time, thinner doped poly-Si layers drastically decrease the FCA but also enable Ag to absorb more light parasitically.

V. CONCLUSIONS

The impact of main process-related parameters on the performance of IBC solar cells featuring poly-Si carrier selective contacts was here studied. Carrier selectivity and tunneling concepts were used to identify the parameters affecting transport in terms of FF. It was identified that carrier density at c-Si/SiO$_2$ interface together with oxide thickness affect the collection of carriers. For an efficient transport, carrier concentrations at interface is supported by in-diffused dopants from highly doped poly-Si layers resulting from high temperature process. Our simulation framework based on TCAD Sentaurus was validated by comparing measured and simulated R, T, and EQE spectra, and electrical parameters of a reference device. As result of the calibration process, the opto-electrical losses were quantitatively and qualitatively identified. Main losses were related to recombination, of which 41% due to the front surface and 51% due to the bulk. The calibrated model was afterwards devoted to analyzing the impact of process parameters on the performance of our reference IBC device. The parameters under study were SiO$_2$ thickness, rear side geometry, and passivation quality at front and rear surfaces. Aiming at exploring the potential conversion efficiency of our architecture, we looked at both the reference device and an ideal device, featuring outstanding bulk lifetime and passivation quality ($\tau_{bulk} = 10$ ms and $SRV = 0.1$ cm$^2$/s) with no FSF. Simulation results revealed that SiO$_2$ thickness beyond 1.6 nm forbids to achieve high efficiency, due to transport degradation ascribed to the strong decrease in tunneling probability of collecting carriers. Indeed, SiO$_2$ thickness < 1.6 nm improves the transport of collecting carriers. On the other hand, SiO$_2$ thickness < 1 nm enables also the transport of non-collecting carriers thus increasing contact recombination. Therefore, we identified an optimum oxide thickness of 1 nm that allows the tunneling of collecting carriers while still concurrently restricting tunneling of non-collecting carriers. For 1-nm thick SiO$_2$, $\eta = 25.9\%$ was calculated. Additionally, we observed that the efficiency curve as function of emitter width exhibits a bell shape with a clear maximum value for a p-type contact width over pitch ratio of 69%. We also found that n-type contact, p-type contact and FSF doping profiles inside c-Si enhance the electrical field passivation. Therefore, $V_{oc}$ and $\eta$ are almost insensitive to SRV values up to $1 \times 10^2$ cm/s in case of BSF and emitter and up to $1 \times 10^3$ cm/s in case of FSF. Keeping 1-nm thick tunneling SiO$_2$, engineering the doping profile of both emitter and BSF and switching from 280-μm to 100-μm thick bulk, the calculated potential conversion efficiency was raised to 26.7%. Following further optimizations that touched upon poly-Si thickness (20 nm), metal contact material (Ag), metallization fraction (80%) and double ARC (SiN$_x$ / MgF$_2$), an ultimate efficiency of 27.3\% was simulated.

Our simulation methodology assumes that transport through uniform thin SiO$_2$ layer is exclusively described by tunneling concepts neglecting pinhole-transport contribution. In particular, the followed modelling approach has been successfully deployed for the design of advanced semiconductor devices and related processes. In this work, we have not performed extensive experimental characterization to assess the applicability of contradicting transport models (tunneling, pinholes or both). Accordingly, presented results should be interpreted considering this assumption in mind.

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VI. REFERENCES


