Amorphous silicon oxide window layers for high-efficiency silicon heterojunction solar cells

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In amorphous/crystalline silicon heterojunction solar cells, optical losses can be mitigated by replacing the amorphous silicon films by wider bandgap amorphous silicon oxide layers. In this article, we use stacks of intrinsic amorphous silicon and amorphous silicon oxide as front intrinsic buffer layers and show that this increases the short-circuit current density by up to 0.43 mA/cm² due to less reflection and a higher transparency at short wavelengths. Additionally, high open-circuit voltages can be maintained, thanks to good interface passivation. However, we find that the gain in current is more than offset by losses in fill factor. Aided by device simulations, we link these losses to impeded carrier collection fundamentally caused by the increased valence band offset at the amorphous/crystalline interface. Despite this, carrier extraction can be improved by raising the temperature; we find that cells with amorphous silicon oxide window layers show an even lower temperature coefficient than reference heterojunction solar cells (−0.1%/°C relative drop in efficiency, compared to −0.3%/°C). Hence, even though cells with oxide layers do not outperform cells with the standard design at room temperature, at higher temperatures—which are closer to the real working conditions encountered in the field—they show superior performance in both experiment and simulation. © 2014 AIP Publishing LLC.

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I. INTRODUCTION

An important prerequisite for reaching high efficiencies in crystalline silicon solar cells is good surface passivation of the wafer. This enables high voltages at open circuit (Voc) but also at the maximum power point, leading to high fill factors (FF). For silicon heterojunction (SHJ) solar cells, intrinsic hydrogenated amorphous silicon (i a-Si:H) buffer layers have been proven to offer outstanding passivation.6,7 In this cell design, shown schematically in Fig. 1, doped (n or p) a-Si:H overlayers are used to form junctions as electron and hole collectors,6,7 allowing the fabrication of nearly recombination-free contacts.2–5 However, the high absorption coefficient and relatively narrow quasi-direct bandgap of a-Si:H (~1.7 eV), combined with its high defect density, give rise to significant parasitic losses in the ultraviolet and visible range of the solar light spectrum, as most of the photogenerated carriers in these films recombine before they can be collected.11–14 For typical SHJ cells, we found earlier that all light absorbed in the p-layer is lost, whereas one-third of the light absorbed in the intrinsic passivation layer contributes to the generation of current.15 Parasitic absorption also occurs in the front transparent conductive oxide (TCO) layer, the presence of which is required for efficient current extraction due to the low lateral conductivity of the doped a-Si:H layers. We currently lose only 0.3 mA/cm² in the front TCO for wavelengths below 600 nm, which is much less than the 2 mA/cm² lost in our standard front a-Si:H layers.15

A possible approach to reduce parasitic absorption also in the a-Si:H layers is to increase the threshold energy for absorption by using a material with a wider bandgap. Wide-bandgap doped amorphous silicon oxide layers with nano-crystallites (nc-SiOx:H) are used in thin-film silicon tandem solar cells as window layers and intermediate reflectors16,17 showing the potential for improved light management. In SHJ devices, intrinsic amorphous silicon oxide (a-SiOx:H) as well as doped nc-SiOx:H layers were tested as passivation and charge-carrier collection layers, respectively, and promising results were reported on p-type18–20 and n-type21...
crystalline silicon wafers. However, a direct comparison of such layers to state-of-the-art a-Si:H films has been lacking so far, making an assessment of their true potential difficult.

In the present work, we make this comparison and focus on introducing \( i \)-a-Si\(_{Ox}:H \) in the place of standard \( i \)-a-Si:H to assess its potential as a buffer and window layer at the front. From the literature it is known that the doping efficiency of a-Si:H is reduced by the introduction of oxygen.\(^{22}\) Hence, to avoid possibly ambiguous results, in this work, we concentrate on the buffer layer only and present studies on how the oxygen content and thickness of the layer influence device performance. We assess the wafer passivation properties of a-Si\(_{Ox}:H\) layers, their optical properties and their influence on carrier collection.

II. EXPERIMENTS

The device results discussed in this work were obtained for 2 \( \times \) 2 cm\(^2\) cells (with 3 cells per wafer) with the following structure (see Fig. 1); screen-printed Ag front grid/indium tin oxide (In\(_2\)O\(_3\):Sn, ITO) 70 nm/p\(^+\) a-Si:H 10 nm/\( i \)-a-Si:H or \( i \)-a-Si\(_{Ox}:H\) (5 nm unless otherwise indicated)/textured float-zone \( n \)-c-Si 230 \( \mu \)m/i-a-Si:H 5 nm/n\(^+\) a-Si:H 10 nm/ITO 150–200 nm/Ag full rear metallization. For fabrication, first the wafers were textured using potassium hydroxide, then they were cleaned by wet-chemical means, and following gases were used: silane (SiH\(_4\)), hydrogen (H\(_2\)), trimethylborane (B(CH\(_3\))\(_3\)), TMB) and phosphine (PH\(_3\)) for doping and carbon dioxide (CO\(_2\)) as the oxygen source. The layers were deposited at 200°C for chemical oxide removal just before layer deposition. All \( i \)-a-Si:H layers were deposited at 200°C in a medium-sized (electrode size: 15 \( \times \) 16 cm\(^2\)) plasma-enhanced chemical vapor deposition (PECVD) cluster tool (INDEOtect, Octopus\(^{TM}\)) with individual chambers dedicated to intrinsic and doped layer deposition. The inter-electrode gap for this system is 15 mm and the chambers are powered at 13.56 MHz. For the layer depositions, mixtures of the following gases were used: silane (SiH\(_4\)), hydrogen (H\(_2\)), trimethylborane (B(CH\(_3\))\(_3\)), TMB) and phosphine (PH\(_3\)) for doping and carbon dioxide (CO\(_2\)) as the oxygen sources. The layers were co-deposited on wafers and glass samples for layer characterization, as will be described later. After PECVD, the effective minority-carrier lifetimes (\( \tau_{\text{eff}} \)) of the cell precursors were measured using a Sinton Consulting WCT-100 quasi-steady-state photoconductance system.\(^{23}\) This measurement was also used to extract the so-called implied \( V_{\text{oc}} \).\(^{23}\) The next step was the deposition of ITO by sputtering on both the front and rear (see Ref. 24 for further details), and the deposition of a silver contact at the rear either by sputtering or evaporation. To finish the cells, the front metallization grid was screen-printed using a low-temperature silver paste, which was subsequently cured on a belt furnace at temperatures below 200°C.\(^{25}\) The entire cell fabrication process used in this work is fully compatible with industrial standards.

The cells were characterized using standard (AM 1.5 G) current-voltage (\( J-V \)) measurements at ambient or higher temperatures (up to the setup limit of 55°C), as well as suns-\( V_{\text{oc}} \) measurements.\(^{26}\) Furthermore, systematic spectral response and reflectance measurements were conducted to determine external quantum efficiency (EQE), reflectance (\( R \)), and internal quantum efficiency (IQE).

Spectroscopic ellipsometry (SE) was used to characterize the layers that were co-deposited on glass. Using a Tauc-Lorentz multi-layer model to fit the data, the refractive index \( n \), the extinction coefficient \( k \), the optical bandgap \( E_{\text{opt}} \) (determined at an absorption coefficient \( \alpha = 10^{4}\ \text{cm}^{-1} \)) and the layer thickness were extracted. Unless stated differently, the layer thicknesses refer to the thicknesses on a textured wafer, i.e., thicknesses measured on a flat substrate (glass) divided by a geometrical factor of 1.7.\(^{1} \)

Thermal desorption spectroscopy (TDS) was used to investigate the bonding configuration of hydrogen within \( i \)-a-Si\(_{Ox}:H\) passivation layers. For this measurement, the sample (typically a piece of c-Si with the layer on top) was heated in ultra-high vacuum and the gases desorbed from it were analyzed by a quadrupole mass spectrometer. More details can be found elsewhere.\(^{27}\)

Furthermore, we used Fourier transform infrared spectroscopy (FTIR) in perpendicular transmittance mode to verify the presence of oxygen for an approximately 95-nm-thick layer. This was done by analyzing the modes of Si-O centered at around 1000 cm\(^{-1}\) and 1150 cm\(^{-1}\) (Ref. 28) as well as the mono-hydride and multi-hydride modes at 2010 cm\(^{-1}\) and 2100 cm\(^{-1}\), respectively (Ref. 29).

III. RESULTS AND DISCUSSION

A. Passivation properties of \( i \)-a-Si\(_{Ox}:H\)

To evaluate the passivation and optical properties of \( i \)-a-Si\(_{Ox}:H\) films, double-side polished, (100), 300-\( \mu \)m-thick phosphorous-doped wafers with a resistivity of 4 \( \Omega \) cm were passivated by 16-nm-thick layer stacks deposited on both sides. These stacks consisted of a very thin \( i \)-a-Si:H layer (~2 nm, from ellipsometry), on which an \( i \)-a-Si\(_{Ox}:H\) layer of varying composition was deposited. This was done since direct deposition of \( i \)-a-Si\(_{Ox}:H\) layers on the wafer surfaces resulted in systematically poor passivation (results not shown). In the remainder of the text, the presence of such thin \( i \)-a-Si:H layers is implicitly assumed. The effective minority-carrier lifetime (\( \tau_{\text{eff}} \)) of each passivated sample was measured both in the as-deposited state as well as after annealing at 200°C for 100 min in air (Fig. 2). The approximate effective surface recombination velocity (\( S_{\text{eff}} \)) was calculated from the following equation for \( \tau_{\text{eff}} \) (with wafer thickness W):

\[
\frac{1}{\tau_{\text{eff}}} = 2 \frac{S_{\text{eff}}}{W}.
\]

Equation (1) assumes symmetric passivation at the front and rear surfaces and a bulk lifetime of \( \tau_{\text{bulk}} \rightarrow \infty \). Excellent as-deposited lifetimes of \( \tau_{\text{eff}} > 5 \) ms (\( S_{\text{eff}} < 3 \) cm/s) are obtained across the entire input gas flow ratio range. Samples passivated by silicon-rich films show a clear further improvement in passivation upon low-temperature annealing, a phenomenon well-known for pure a-Si:H films.\(^{30}\) The samples fabricated with CO\(_2)/\text{SiH}_4 \) gas flow ratios higher than 0.8 show a slightly lower \( \tau_{\text{eff}} \) and a smaller increase in
Passivation quality upon annealing compared to the samples fabricated at lower CO\textsubscript{2}/SiH\textsubscript{4} gas flow ratios (Fig. 2).

One possible explanation for this slight drop in passivation quality may be the increasingly porous character of the layers. An indication of such porosity was observed by TDS measurements, they showed that by adding oxygen to the layer its passivation quality upon annealing compared to the samples fabricated at lower CO\textsubscript{2}/SiH\textsubscript{4} gas flow ratios (Fig. 2).

Here, for an increasing CO\textsubscript{2}/SiH\textsubscript{4} ratio, a mono-hydrides and for the presence of hydrogenated voids measurements were normalized to the volume of the respective layers. The trend lines are guides for the eye.

FIG. 2. Effective minority-carrier lifetimes (at an excess carrier density of \(\Delta n = 10^{15} \text{cm}^{-3}\)) before and after annealing for 100 min at 200 °C in air for \(n\)-type float-zone wafers passivated with approximately 16-nm-thick \(i\) a-Si\textsubscript{O\textsubscript{x}}:H stacks deposited with different CO\textsubscript{2}/SiH\textsubscript{4} input flow ratios. The trend lines are guides for the eye.

FIG. 3. (a) TDS data of H\textsubscript{2} (\(m/\epsilon = 2\)) taken for \(i\) a-Si\textsubscript{O\textsubscript{x}}:H layers deposited directly on polished wafers, i.e., without an \(i\) a-Si:H layer beneath. The measurements were normalized to the volume of the corresponding layer and the curves are offset for clarity. The arrows indicate the range used for integration (200–800 °C). (b) Relative H\textsubscript{2} increase for the layers shown in (a), normalized to the layer deposited with CO\textsubscript{2}/SiH\textsubscript{4} = 0.4.
approximately 94-nm-thick layer deposited on a double-side polished (100) wafer at a CO2/SiH4 gas ratio of 2.5 was confirmed by FTIR measurements. In contrast to our standard i-layers,43 we observed a significantly higher absorbance for the mode centered around 2100 cm$^{-1}$ compared to the mode at 2000 cm$^{-1}$ (Fig. 5). This points to more hydrogen-terminated voids, which confirms our results obtained from TDS. Note that compared to the standard i-a-Si:H layer, the spectrum for the i-a-SiOx:H layer exhibits additional peaks at higher wavenumbers (SiH(O3), SiH2(O2), and SiH2(SiO), Fig. 5). These can be attributed to oxygen present in the layer.44 Both the increasing amount of hydrogen and—for our case, to a minor extent—oxygen may lead to an increasing valence band (VB) offset.41,45 This can explain the significant effect on carrier collection we observe in our devices, which will be discussed in Sec. III.C.

To assess the potential current gain ($\Delta J_{eq}$) that can be expected with such wider bandgap films, we used the $n$ and $k$ values as input for OPAL46 simulations. The parasitic absorption in a device-relevant stack of ITO (70 nm), $p^+$ a-Si:H (6 nm) and i-a-Si:H or i-a-SiOx:H (6 nm) on a textured wafer was calculated for different oxygen contents. We then determined an equivalent short-circuit current density ($J_{eq}$) lost through parasitic absorption in the three front layers by integrating the product of absorption and photon flux (standard AM 1.5 G spectrum) from 300 to 600 nm and 600 to 1200 nm. We thereby obtained a potential total gain of up to 0.81 mA/cm$^2$ (300–600 nm: 0.51 mA/cm$^2$, 600–1200 nm: 0.31 mA/cm$^2$) for a layer deposited at a CO2/SiH4 ratio of 2.5 (Fig. 4(c)). We attribute this gain to an increase of the bandgap and—for our case, to a minor extent—oxygen may lead to an increasing valence band (VB) offset.41,45 This can explain the significant effect on carrier collection we observe in our devices, which will be discussed in Sec. III.C.

In a next step, we fabricated solar cells and implemented either standard i-a-Si:H (both sides, standard cell) or i-a-SiOx:H (front only) passivation layers. We varied both the CO2/SiH4 gas flow ratio and the layer thickness, and we obtained an increase of approximately 0.43 mA/cm$^2$ for ~6-nm-thick a-SiOx:H passivation layer deposited at CO2/SiH4 = 2.5. Comparing the EQE and IQE data of both cells, the gain in the range of 300–600 nm is of 0.27 mA/cm$^2$ while for the range 600–1200 nm we see a gain of 0.29 mA/cm$^2$, which amounts to a total gain of 0.56 mA/cm$^2$.47 The fact that the increase in current is a result of the widening bandgap and an anti-reflective effect is confirmed by these results from real devices (Figs. 6(a)–6(d)). While $R$ at 400 nm is constant for the standard a-Si:H layers—which have nearly the same $n$ as c-Si—as their thickness is increased, we see a decrease in $R$ for all of the a-SiOx:H layers. This explains why the EQE (at 400 nm) of the cells with oxide layers shows only a weak thickness dependence (Fig. 6(b); parasitic absorbance increases but $R$ decreases), whereas we see a strong dependence for the standard a-Si:H layers.

C. Application of i-a-SiOx:H in solar cells

Figure 7 shows the illuminated $J-V$ parameters of solar cells featuring i-a-SiOx:H buffer layers of various thickness and composition. Some of the $J-V$ curves are strongly s-shaped and the voltage measured at zero current (in some cases above 830 mV) exceeds the theoretical limit48 for c-Si.1 Hence, rather than showing the 1-sun $V_{oc}$ values, we show the implied $V_{oc}$ values obtained from lifetime measurements as an indication of the level of passivation. Also, in devices, the CO2/SiH4 ratio has only a minor influence on the passivation quality (Fig. 7(a)), which is high for all of the cells, as evidenced by the implied $V_{oc}$ values in excess of 720 mV.
CO2/SiH4 ratio is most likely due to the change in the band offset at the a-Si:H/a-SiOx:H interface41 and is in agreement with findings by Shu et al.50 Using simulations, they linked a decrease in FF to an increase in buffer layer bandgap. In our case, collecting holes at the front, an increased VB offset at the interface between the wafer and buffer layer may be especially detrimental, as the holes face a higher effective barrier than electrons would (namely, the conduction band (CB) offset), making their collection less efficient.

To assess the influence of this barrier on hole transport, we conducted J-V measurements on a standard cell (i a-Si:H buffer, ~6 nm thick, Fig. 8(a)) and a cell with an a-SiOx:H passivation layer (CO2/SiH4 = 0.8, ~6 nm thick, Fig. 8(b)) at different temperatures. When increasing the temperature from 25°C to 55°C, the Voc decreases by roughly 50 mV for both cells due to an increase in dark saturation current density through the increase of the intrinsic carrier density (ni).

However, compared to the reference, the a-SiOx:H cell shows a slightly lower absolute value of the relative change in Voc, −0.22%/°C instead of −0.25%/°C (data not shown). Furthermore, besides this effect, the standard cell shows a decrease in FF of approximately 2% absolute, whereas the cell with an oxide layer recovers almost 2% for the same temperature range (Fig. 8(e)). This improvement confirms earlier findings for wide-bandgap a-Si:C:H buffer layers.50 Due to a more favorable (efficiency) temperature coefficient β ~ −0.1%/°C (compared to −0.3%/°C for the reference) in the investigated temperature range, the cell with an implemented oxide buffer layer shows an efficiency which, at high temperatures—those closer to real working conditions in the field—is superior to the standard cell design (Fig. 9). At 55°C, the cell with an oxide buffer layer exhibits an efficiency of 18.0% (18.6% at 25°C), compared to 17.7% (19.6% at 25°C) obtained from the reference cell. A similar effect has been reported in a simulation study by Rahmouni et al.,51 where thicker buffer layers lead to favorable temperature coefficients due to improving FF. However, in contrast to our findings for a-SiOx:H layers, devices with thicker i a-Si:H passivation layers do not show a better performance at elevated temperatures. Their efficiencies stay below the efficiency of the reference device with a 3-nm-thick i a-Si:H layer.

FIG. 7. (a) Implied open-circuit voltage, (b) short-circuit current density, (c) fill factor (the dashed lines are linear fits to the data) and (d) cell efficiency as a function of the front i-layer thickness (on textured wafers). The data points represent the average of three cells on the same wafer. The error bars indicate the standard error of the mean. Note that the series at a ratio of 0.8 featured a different batch of wafers, i.e., different cleaning and texturization, than the others; hence the slight differences in implied open-circuit voltage.

FIG. 8. (a), (b) J-V measurements (temperature: 25–55°C in steps of 10°C) and (c), (d) simulations (25–85°C, in steps of 10°C) for devices with an i a-Si:H or i a-SiOx:H front passivation layer. The arrows indicate the increasing temperature and illustrate the different behaviors. (e) FF evolution with temperature (filled symbols: J-V measurements, open symbols: simulation) for both cells. (f) PC1D52 simulation of the energy bands close to the a-SiOx:H/c-Si interface in short-circuit (sc), at maximum power point (mpp) and in open-circuit (oc) conditions.
To better understand the observed trends in FF for our devices, one-dimensional device simulations were carried out using the software packages SunShine$^{53}$ and ASPIN$^{54}$ for the optical and electrical models, respectively. To obtain the generation-rate profile throughout the cell, a 70-nm-thick front ITO layer (anti-reflective coating) and a 150-nm-thick rear ITO layer with 300 nm of Ag (rear reflector) were added. The simulations were done on flat layers, yet in order to simulate a textured wafer and match the measured J-V data of the relevant layers obtained from SE were used.$^{55}$

For electrical simulations, the surface defect density at both the front and rear a-Si:H/c-Si interfaces was set to $5 \times 10^{10}$ cm$^{-2}$ to match the measured $V_{oc}$. The parameters of the different materials were chosen as described in Table I. We assumed the same electron affinity for all of the amorphous layers, i.e., only the VB offset$^{41}$ varied upon changing the bandgap of the a-SiO$_x$:H layer from 1.7 eV to 1.9 eV, whereas the CB offset remained constant. This reflects the assumption we made that mainly the VB position changes upon hydrogen incorporation and widening of the bandgap. For simplicity, only thermionic emission across the barrier was included in the simulations; neither the temperature dependence of the bandgaps, Auger recombination, nor tunneling at the heterointerface was taken into account.

Figures 8(c) and 8(d) show the simulated J-V curves (25–85 °C, step size of 10 °C) corresponding to the measured J-V curves in Figures 8(a) and 8(b) (25–55 °C, step size of 10 °C). Remarkably, similar trends were obtained with the simulations, especially for the FF (Fig. 8(e)). We therefore conclude that the drop in FF we observed in cells with thin a-SiO$_{x}$:H passivation layers must indeed be a result of impeded hole collection due to a higher VB offset$^{51,56}$ which leads to an accumulation of holes.$^{57}$ The effect depends on the working point of the device and becomes more significant when moving from short-circuit to open-circuit conditions. In short-circuit conditions, there is strong band bending, as indicated in Fig. 8(f). Therefore, holes are easily collected across the junction thanks to a high electric field, and hole accumulation at the interface is kept low. However, moving towards open-circuit conditions, the bands flatten (Fig. 8(f)), and the accumulation of holes at the interface increases. It has been reported that this accumulation of holes at the interface can lead to a strong increase of recombination and thus to a reduction of the photocurrent$^{58}$ and thus, in our case, of the FF. This effect is one possible explanation for the behavior we obtain for our devices.

The increase in FF with temperature observed for cells with a-SiO$_{x}$:H buffer layers points then to enhanced carrier transport, probably due to thermionic emission of the holes over the barrier at maximum power point. We remark that optimized standard devices are considered to operate in a carrier-diffusion-limited regime, very similar to homojunction devices (Ref. 59). In this case, the decrease in FF with increasing temperature is likely a consequence of the standard temperature-induced drop in voltage at the maximum-power point. This is most likely linked to the detrimental temperature dependency of the dark saturation current density. The increase in line resistance with temperature plays only a negligible role due to the small resistivity temperature coefficient of silver.

In order to investigate further the influence of the VB offset, we performed another set of simulations using the same model as described before (a-SiO$_{x}$:H cell, Table I). However, this time we varied the electron affinity (E$_{a}$, Fig. 10(d)) of the i a-SiO$_{x}$:H buffer layer while keeping the other parameters fixed. Changing its value from 3.72 eV to 3.92 eV, both the CB and VB edge move down in energy and the VB offset increases by 0.2 eV from (1) that of the reference cell to (2) that assumed for the oxide cell (Fig. 10(a)). This has the same effect on the FF as we observed in our experiments when increasing the CO$_2$/SiH$_4$ ratio and confirms that it is the VB offset that hinders the carriers from being collected efficiently and that lowers FF at room temperature. To further underline this fact, two additional series of simulations were performed. This time the VB offset was fixed to the values of positions (1) and (2) in Fig. 10(a) and the CB offset was varied by changing both the electron affinity and the bandgap at the same time (Figs. 10(b) and 10(c)).

TABLE I. Parameters used for simulations of a standard cell with an a-Si:H passivation layer, and of a cell with an a-SiO$_{x}$:H front passivation layer.

<table>
<thead>
<tr>
<th>Layer</th>
<th>p a-Si:H</th>
<th>n a-Si:H</th>
<th>i a-Si:H/a-SiO$_{x}$:H</th>
<th>c-Si</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thickness</td>
<td>10 nm</td>
<td>10 nm</td>
<td>8.5 nm</td>
<td>230 µm</td>
</tr>
<tr>
<td>Bandgap (eV)</td>
<td>1.7</td>
<td>1.7</td>
<td>1.7/1.9</td>
<td>1.124</td>
</tr>
<tr>
<td>Electron affinity (eV)</td>
<td>3.924</td>
<td>3.924</td>
<td>3.924</td>
<td>4.05</td>
</tr>
<tr>
<td>Doping concentration (cm$^{-3}$)</td>
<td>$1 \times 10^{19}$</td>
<td>$1 \times 10^{19}$</td>
<td>0</td>
<td>$1.2 \times 10^{15}$</td>
</tr>
<tr>
<td>Electron/hole mobility (cm$^2$/Vs)</td>
<td>10/2</td>
<td>10/2</td>
<td>10/2</td>
<td>1320/450</td>
</tr>
</tbody>
</table>
For both cases, the $FF$ shows only a weak dependence on the CB offset value. Therefore—even though an increase in CB offset or additional effects lowering the $FF$ cannot be excluded completely—we believe that it is the VB offset which mainly limits carrier (hole) transport.

IV. BEST CELL RESULTS

Combining our findings, and following further optimization, our best cell with an a-SiO$_x$:H passivation layer at the front (CO$_2$/SiH$_4$ = 0.4) showed a $V_{oc}$ of 716 mV, a $J_{sc}$ of 37.1 mA/cm$^2$, a $FF$ of 76.8% and an efficiency of 20.4% (Fig. 11, dashed line). Although the $J_{sc}$ increased by approximately 0.2 mA/cm$^2$ by using an a-SiO$_x$:H passivation layer, the cell efficiency at room temperature decreased due to an absolute reduction in $FF$ of 1.7%. Based on our device simulations, this limitation is likely to be fundamental, where an increase in $J_{sc}$ by opening the bandgap of the buffer layer, and thereby increasing the VB offset, will be compensated by a drop in $FF$ resulting from impeded collection of holes.

V. CONCLUSIONS

We compared devices with a-SiO$_x$:H passivation layers at the front to devices with standard a-Si:H passivation layers. No significant difference in passivation was observed and comparable implied $V_{oc}$ values of around 725 mV were obtained. An increase in bandgap and a simultaneous decrease in short-wavelength reflection were observed with oxide layers. Both lead to an increase in $J_{sc}$ of up to 0.43 mA/cm$^2$ for CO$_2$/SiH$_4$ = 2.5. Despite this gain—at room temperature—the expected improvement in efficiency is more than compensated for by losses in $FF$. Using simulations, we linked the $FF$ losses to an increased VB offset at the interface between the amorphous and crystalline phases, which results in a blockade for holes. This raises concerns whether wider bandgap window layers offer potential for improved device performance. Nevertheless, under the condition that it shows a good passivation quality and that the band lineup does not impede the carrier collection, a wide-bandgap buffer layer can be used. If the device will operate at elevated temperatures, the present design may be employed, as we found that a wide bandgap a-SiO$_x$:H buffer layer leads to a smaller absolute value of the temperature coefficient and to superior performance at elevated temperature compared to the standard cell. We note that, in many cases, the working conditions for a module in the field are actually far above room temperature, so the potential of these cells is obvious, especially for warmer climates.

Conversely, it may be preferable to collect electrons at the a-SiO$_x$:H buffer layer side, as the larger VB offset should not impede electrons. In that case, the cell architecture should be redesigned towards a rear-emitter cell (when using n-type wafers). Otherwise, the polarity of the complete device needs to be changed by using p-type wafers and n-type electron collecting layers at the front.

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FIG. 10. (a) $FF$ as a function of the change in VB offset (variation of $\Delta E_v$). At position (1), the VB offset corresponds to the offset of the reference cell, whereas at position (2), it is approximately equal to the offset of the cell with an oxide buffer layer. (b) and (c) show the $FF$ as a function of the change in CB offset (variation of $\Delta E_C$), keeping the VB offset constant at positions (1) and (2), respectively. (d) Schematic band diagram illustrating the energies varied in the simulations (electron affinity $E_a$ and vacuum level $E_{vac}$).

FIG. 11. Illuminated $J$-$V$ measurements of our best 2 x 2 cm$^2$ cells in these experiments, measured in house under standard test conditions.