Transparent silicon carbide/tunnel SiO₂ passivation for c-Si solar cell front side: Enabling $J_{sc} > 42 \text{ mA/cm}^2$ and $iV_{oc}$ of 742 mV

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Abstract

N-type microcrystalline silicon carbide ($\mu$-SiC:H(n)) is a wide bandgap material that is very promising for the use on the front side of crystalline silicon (c-Si) solar cells. It offers a high optical transparency and a suitable refractive index that reduces parasitic absorption and reflection losses, respectively. In this work, we investigate the potential of hot wire chemical vapor deposition (HWCVD)–grown $\mu$-SiC:H(n) for c-Si solar cells with interdigitated back contacts (IBC). We demonstrate outstanding passivation quality of $\mu$-SiC:H(n) on tunnel oxide (SiO₂)–passivated c-Si with an implied open-circuit voltage of 742 mV and a saturation current density of 3.6 fA/cm². This excellent passivation quality is achieved directly after the HWCVD deposition of $\mu$-SiC:H(n) at 250°C heater temperature without any further treatments like recrystallization or hydrogenation. Additionally, we developed magnesium fluoride (MgF₂)/silicon nitride (SiNₓ:H)/silicon carbide antireflection coatings that reduce optical losses on the front side to only 0.47 mA/cm² with MgF₂/SiNₓ:H/$\mu$-SiC:H(n) and 0.62 mA/cm² with MgF₂/$\mu$-SiC:H(n). Finally, calculations with Sentaurus TCAD simulation using MgF₂/$\mu$-SiC:H(n)/SiO₂/c-Si as front side layer stack in an IBC solar cell reveal a short-circuit current density of 42.2 mA/cm², an open-circuit voltage of 738 mV, a fill factor of 85.2% and a maximum power conversion efficiency of 26.6%.

Keywords
antireflecting coating, excellent passivation, heterojunction, hot wire CVD, lean process, refractive index, silicon carbide, tunnel oxide
1 | INTRODUCTION

Crystalline silicon (c-Si) solar cells have reached energy conversion efficiencies above 26%,1,2 with the help of full area selective passivating contacts. For such high conversion efficiencies, intrinsic amorphous silicon (a-Si:H(i)) and ultrathin tunnel oxide (SiO2) have become the predominant materials for the passivation of c-Si surfaces.3 A comparison of both passivation concepts shows that record cells with a-Si:H(i) passivation developed for the silicon heterojunction (SHJ) technology currently give rise to higher open-circuit voltages (Voc) than using SiO2 passivation7 from polycrystalline silicon on oxide (POLO) technology or tunnel oxide passivating contact (TOPCon) technology. Further, for a-Si:H(i), the excellent interface passivation is directly achieved after the deposition of the a-Si:H(i) film, whereas for SiO2, it requires several additional process steps to provide excellent interface passivation.4 Reducing the number of process steps is under current investigation within several research groups in the field of c-Si solar cells. Although a-Si: H(i) is an excellent passivation material, it possesses an optical bandgap5 of approximately 1.7 eV that leads to significant parasitic absorption of the incident sunlight.

N-type microcrystalline silicon carbide (μc-SiC:H(n)) grown by hot wire chemical vapor deposition (HWCDV) is known for its large optical bandgap—6–7 of 2.4 to 3.4 eV. This high optical transparency makes it a promising window layer material,5 which was developed for silicon thin-film solar cells9 as well as for silicon heterojunction solar cells,7,10 However, the deposition conditions for growing highly transparent μc-SiC:H(n) on top of a-Si:H(i) lead to strong deterioration of the underlying amorphous silicon layers, because of etch-off of the films.6,8,11 This trade-off between high-quality passivation and attractive transparency has limited the beneficial implementation of μc-SiC:H(n) in silicon solar cells for a long time. In the past, we showed that it is possible to fabricate symmetric test structures, where the layer stack of HWCDV-grown μc-SiC:H(n) on tunnel SiO2 passivated the c-Si surfaces. We achieved high passivation quality with implied open-circuit voltages (Voc) of up to 728 mV and saturation current densities (J0) down to 7.1 fA/cm2 on double-side textured c-Si wafers.7,12 We further reported on the corresponding contact resistivities derived in the cited references, where the lowest value7 was 18 mΩcm2. These promising results were achieved directly after the HWCDV deposition of μc-SiC:H(n) and without any further treatments, eg, annealing or hydrogenation. Because of the large optical bandgap of μc-SiC:H(n), we named the layer stack of μc-SiC:H(n)/SiO2/c-Si transparent passivating contact (TPC) in the past.7,12

So far, the TPC was only used for two side contacted c-Si solar cells,7,12 where it replaced the a-Si n-layer and i-layer of the front side by transparent μc-SiC:H(n)/SiO2. Additionally, it is possible to contact the TPC with indium tin oxide and conventional low-temperature screen-printed silver contacts, in order to use it as a font side c-Si solar cell concept.

In this work, we investigate the potential of the transparent μc-SiC:H(n)/SiO2 passivation layer stack used as part of an antireflection coating (ARC) for the front side of a c-Si solar cell with interdigitated back contacts (IBC) as illustrated in Figure 1. The concept of IBC offers the possibility to achieve the highest short-circuit current densities (Jsc), because of the absence of shading metal contacts on the front side. We developed an ARC consisting of magnesium fluoride (MgF2), silicon nitride (SiNx:H), and μc-SiC:H(n) as illustrated in Figure 1. For that purpose, it was important to tune the thickness of μc-SiC:H(n) for a minimum total optical loss of parasitic absorption and reflection.

The Jsc of the currently best silicon-based solar cells are 42.9 mA/cm2 for Fraunhofer ISE TOPCon,13 42.7 mA/cm2 for Kaneka SHJ-IBC,1 42.6 mA/cm2 for ISFH POLO-IBC2 and 42.7 mA/cm2 for UNSW PERL.14 All Jsc values of the record cells are above 42 mA/cm2, but they were either achieved by many process steps or undisclosed fabrication processes. Thus, the goal of this work was to develop a transparent passivation as part of an ARC for the front side of IBC c-Si solar cells using a lean process flow that gives rise to very high Jsc values above 42 mA/cm2.

2 | EXPERIMENTAL DETAILS

The μc-SiC:H(n) layers were deposited in an HWCDV vacuum chamber with three curved rhenium wires, 6-sccm flow rate of the monomethylsilane (MMS) gas, which is diluted to 5% in H2, 94-sccm flow rate of the H2 gas, 75-Pa chamber pressure, 250°C heater temperature, and 1800°C filament temperature. SiNx layers were deposited in a plasma-enhanced chemical vapor deposition chamber using 7.8 sccm of SiH4 and 10 sccm of NH3 diluted in 450 sccm of Argon and 138 sccm of Helium. The chamber pressure was 8 Pa, the heater temperature was 100°C, and the inductive coupled plasma power was 700 W. MgF2 layers were thermally evaporated at room temperature. All films were deposited on glass substrates (Corning, EAGLE XG). We derived the complex refractive index for the 130 nm μc-SiC:H(n) film by fitting the reflectance and transmittance spectra with the SCOUT software.15 The reflectance and transmittance...
spectra were measured with a PerkinElmer Lambda 950 UV-Vis spectrophotometer.

Lifetime samples and ARC samples were processed onto double-side textured, phosphorus-doped, Czochralski grown, and <100>-orientated c-Si wafers with a resistivity of 1.0 Ω cm and a thickness of 170 μm. The wafers were cleaned using complete RCA (Radio Corporation of America) treatment. After dipping in diluted hydrofluoric acid (HF) for 10 minutes to remove the oxide, the tunnel oxide was grown for 10 minutes on both sides of the wafer in a piranha solution (H₂O₂: H₂SO₄) at 60°C. Details of the wet-chemical preparation can be found elsewhere. According to spectroscopic ellipsometer measurements of the tunnel oxide on flat <111> orientated wafer the SiO₂ thickness was approximately 1.2 nm. For lifetime samples, the μc-SiC:H(n) layers had a thickness of 30 nm. The thickness, the complex refractive index, and the extinction coefficient of SiNₓ and MgF₂ were obtained by using the SENTECH SE-800 ellipsometer.

The reflectance spectra of the ARC samples were recorded using the LOANA measurement system from pv tools. To simulate optical losses for different ARC stack designs, we used OPAL2 software provided by PV Lighthouse with the measured complex refractive indices of the thin films as input parameters. For the c-Si surface morphology, we assumed randomly distributed, upright pyramids with a characteristic angle of 54.75° as confirmed by SEM images, and a planar fraction of 8%. For the light trapping model, we assumed a substrate thickness of 170 μm. Lastly, potential short-circuit current densities were calculated by means of Monte Carlo ray tracing technique in combination with the transfer matrix method boundary conditions within Sentaurus TCAD. Models and parameters are detailed elsewhere. To highlight the effect of proposed front ARC, we performed the numerical simulations using optimized layer stacks and rear side geometry as described in Procel et al but adapted for 170-μm-thick c-Si wafer with a resistivity of 1 Ω cm.

3 | RESULTS

Before the development of an excellent ARC using HWCVD grown μc-SiC:H(n) for IBC-SHJ solar cells, symmetric test structures of μc-SiC:H(n)/SiO₂/c-Si(n)/SiO₂/μc-SiC:H(n) were fabricated to optimize the passivation of the c-Si surface. The thickness of the μc-SiC:H(n) films was in the range of 30 to 40 nm. The effective charge carrier lifetimes as a function of minority carrier density of two identically prepared samples with the best passivation quality are shown in Figure 2. The corresponding IV_{oc} values at 1 sun illumination are 742 mV for both samples. The values for J₀ are 3.6 and 3.7 fA/cm². Although, after HF-dipping of the test structures, the passivation quality in terms of IV_{oc} and J₀ is unchanged, the growth of an additional SiNₓ:H or MgF₂ layer deteriorates the passivation quality significantly. However, it can be restored by annealing of the sample at 230°C for 20 minutes on a hot plate.

To develop the MgF₂/SiNₓ:H/μc-SiC:H(n) ARCs, the refractive indices (n) and the extinction coefficients (k) were derived from ellipsometry and UV-Vis-spectroscopy, respectively, for μc-SiC:H(n), SiNₓ:H, and MgF₂. The results are plotted in Figure 3 as a function of wavelength together with n and k of c-Si and a-Si:H(n). The full sets of n and k data for μc-SiC:H(n), SiNₓ:H, and MgF₂ can be found in the Supporting Information S1, S2 and S3 [Colour figure can be viewed at wileyonlinelibrary.com]
same wavelength range $n$ is 3.6 to 6.9 for c-Si and 3.1 to 4.9 for a-Si. The extinction coefficients derived for MgF$_2$ and of SiN$_x$:H are zero over the whole wavelength range. For $\mu$c-SiC:H$(n)$, the edge of $k$ ($k = 10^{-4}$) is at 520 nm, while it is at 750 to 760 nm for a-Si and at 1050 nm for c-Si. The full sets of $n$ and $k$ data for $\mu$c-SiC:H$(n)$, SiN$_x$:H, and MgF$_2$ can be found in the Supporting Information.

Using the obtained refractive indices as input parameters for OPAL2 simulations, the spectral reflectance of the MgF$_2$/SiN$_x$:H/$\mu$c-SiC:H$(n)$/SiO$_2$/c-Si stack was calculated for different thicknesses of $\mu$c-SiC:H$(n)$ ($d_{\text{SiC}} = 0$-60 nm). The thickness of MgF$_2$ was kept constant at 100 nm, and SiN$_x$:H thickness was varied between 50 and 60 nm. To be able to compare these results, we fabricated all the triple-layer stacks and measured the reflectance. The results of the simulated reflectance can be found in Figure 4A, while the results of the measured reflectance are shown in Figure 4B. In order to deposit the exact thickness of each layer, the individual thicknesses were adjusted from a reference sample beforehand, using the cross section pictured by scanning electron microscopy (Figure 4C) for thickness measurement of the layers. The resulting simulated and measured reflectance spectra are in very good agreement with each other.

To quantify the reflection losses, we multiplied the simulated and measured reflectance spectra of Figure 4 with the AM1.5 sun spectrum and integrated the result from 300- to 990 nm wavelength. The results are current density losses of $J_{\text{sc}}$ due to reflection as a function of $d_{\text{SiC}}$ (Figure 5). We observe that the simulated reflection current density loss ($J_{\text{sim,R}}$) decreases from 0.45 to 0.14 mA/cm$^2$ by increasing the $d_{\text{SiC}}$ from 0 to 40 nm. For $d_{\text{SiC}}$ larger than 40 nm $J_{\text{sim,R}}$ increases. For the current density losses that were derived from reflectance spectra of the fabricated ARC samples ($J_{\text{meas,R}}$), we observe the same trend. The $J_{\text{meas,R}}$ decreases from 0.42 to 0.13 mA/cm$^2$ by increasing the $d_{\text{SiC}}$ from 0 to 40 nm. The difference between $J_{\text{sim,R}}$ and $J_{\text{meas,R}}$ is within the error range. We further show the simulated parasitic absorption current density loss ($J_{\text{sim,abs}}$) in Figure 5 that was calculated from the extinction coefficient of $\mu$c-SiC:H$(n)$. We observe that $J_{\text{sim,abs}}$ increases from 0 to 0.28 mA/cm$^2$ for $d_{\text{SiC}}$ increasing from 0 to 60 nm. Summing reflection and absorption current densities, the lowest simulated total current density loss is 0.32 and 0.31 mA/cm$^2$ for the measured case, both at $d_{\text{SiC}}$ of 30 nm.

For more sophisticated evaluation of the front side cell design, a state-of-the-art IBC-SHJ-solar cell was simulated using Sentaurus TCAD for the following front side concepts:

i. 108 nm MgF$_2$/75 nm SiN$_x$:H/30 nm $\mu$c-SiC:H$(n)$,
ii. 108 nm MgF₂/30 nm μ-c-SiC:H(n),

iii. 60 nm SiNx:H/10 nm SiO₂.

The resulting reflectance spectra are shown in Figure 6 together with measured reflectance spectra from fabricated samples and resulting spectra from OPAL2 and TCAD simulations. In background, the part of the AM1.5G sun spectrum is indicated, which should be transmitted through the front side layers to be absorbed by the c-Si [Colour figure can be viewed at wileyonlinelibrary.com]

![Figure 6](image)

**TABLE 1** Optical losses of ARC concepts simulated by Sentaurus TCAD

<table>
<thead>
<tr>
<th>ARC Concepts</th>
<th>Front Parasitic Absorption Loss, mA/cm</th>
<th>Front Reflection Loss, mA/cm²</th>
<th>Total Front Loss, mA/cm²</th>
</tr>
</thead>
<tbody>
<tr>
<td>108 nm MgF₂/75 nm SiNx:H/30 nm μ-c-SiC:H(n)</td>
<td>0.15</td>
<td>0.32</td>
<td>0.47</td>
</tr>
<tr>
<td>108 nm MgF₂/30 nm μ-c-SiC:H(n)</td>
<td>0.15</td>
<td>0.47</td>
<td>0.62</td>
</tr>
<tr>
<td>60 nm SiNx:H/10 nm SiO₂</td>
<td>0.21</td>
<td>0.88</td>
<td>1.09</td>
</tr>
</tbody>
</table>

Notes. Corresponding reflectance spectra are shown in Figure 6.

**TABLE 2** Solar cell parameters for different ARC concepts calculated from Sentaurus TCAD simulation for low-cost c-Si wafer with a bulk lifetime of 12 milliseconds

<table>
<thead>
<tr>
<th></th>
<th>108 nm MgF₂/75 nm SiNx:H/30 nm μ-c-SiC:H(n)</th>
<th>108 nm MgF₂/30 nm μ-c-SiC:H(n)</th>
<th>60 nm SiNx:H/10 nm SiO₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jsc, mA/cm²</td>
<td>42.18</td>
<td>42.24</td>
<td>41.84</td>
</tr>
<tr>
<td>Voc, mV</td>
<td>738</td>
<td>738</td>
<td>738</td>
</tr>
<tr>
<td>FF, %</td>
<td>85.19</td>
<td>85.19</td>
<td>85.18</td>
</tr>
<tr>
<td>η, %</td>
<td>26.51</td>
<td>26.55</td>
<td>26.29</td>
</tr>
</tbody>
</table>

The resulting solar cell parameters of all three cases, which were obtained from Sentaurus TCAD simulation, are summarized in Table 2. For the simulations, a charge carrier lifetime in the c-Si bulk (τbulk) of 12 milliseconds was assumed, which corresponds to high-quality wafer. The main difference between the cases was found in Jsc, which is highest for (ii) the MgF₂/μ-c-SiC:H(n) stack (42.24 mA/cm²), followed by (i) the MgF₂/SiNx:H/μ-c-SiC:H(n) stack (42.18 mA/cm²), and is lowest for (iii) the SiNx:H/SiO₂ reference stack (41.84 mA/cm²). For τbulk = 2 ms, which corresponds to cheap low-quality wafer, the solar cell parameters are smaller. For an IBC solar cell with (ii) the MgF₂/μ-c-SiC:H(n) ARC front side, this decreases the results in power conversion efficiency (η) to 25.2%, Jsc to 42.0 mA/cm², open-circuit voltage (Voc) to 733 mV, and fill factor (FF) to 82.1%.

4 | DISCUSSION

Wide bandgap μ-c-SiC:H(n) used on top of a wet-chemically grown silicon tunnel oxide shows the ability to reach Voc > 740 mV and Jsc < 4 fA/cm². This impressive passivation was achieved on double-side textured, phosphorus-doped, Czochralski grown c-Si wafers with a resistivity of 1.0 Ωcm and a thickness of 170 μm. The Voc values are close to the best Voc values reported so far for SHJ technology, where the best values are currently at 744 mV for wafers with...
For a wafer thickness of 165 μm, the estimated practical limit for $i_{sc}$ is 748 mV according to Yoshikawa et al.\textsuperscript{23} To achieve such values close to the practical limit, Taguchi et al\textsuperscript{22} claim that an ultraclean surface is needed, which was not assured for the sample preparation of this work as the HWCVD growth of μc-SiC:H:H(n) was not performed in a clean room. Compared with TOP-Con/POLO technology, the $J_0$ values of μc-SiC:H(n)/SiO$_2$ passivation are among the lowest $J_0$ values reported in the recent past for wet-chemically grown oxides ranging\textsuperscript{13,24} from 1.5 to 20 fA/cm$^2$\textsuperscript{13,24-27}. The improvement in μc-SiC:H(n)/SiO$_2$ passivation as compared with our former work\textsuperscript{7} was achieved by a convolution of an improved surface texture of the c-Si wafer, higher c-Si bulk lifetime, and optimized HWCVD process for the μc-SiC:H(n) deposition. It is important to notice that this excellent level of passivation only requires wet-chemical oxidation and HWCVD deposition of μc-SiC:H(n), which makes it a very simple and lean fabrication process. No further hydro-μc-chemistry and HWCVD deposition of μc-SiC:H(n), which makes it a very simple and lean fabrication process. No further hydro-

**5 | CONCLUSION**

In this study, the potential of a new passivation and antireflection layer stack for IBC solar cells was investigated. The passivation stack consists of a thin wet-chemically grown SiO$_2$ and HWCVD deposited wide bandgap μc-SiC:H(n) on top. Excellent passivation properties with a reproducible $i_{sc}$ of 742 mV and $J_0$ of 3.6 fA/cm$^2$ were achieved directly after the HWCVD deposition of μc-SiC:H(n), without any further treatments like recrystallization or hydrogenation. Because of its high transparency and its suitable refractive index, we developed MgF$_2$/μc-SiC:H(n) and MgF$_2$/SiN$_x$:H/μc-SiC:H(n) stacks as front side ARC for IBC solar cells. Both layer stacks showed very low reflectance that reduced the total optical losses of the front side in short-circuit current density to only 0.62 and 0.47 mA/cm$^2$, respectively. Finally, we simulated a solar cell with state-of-the-art IBC and with MgF$_2$/μc-SiC:H(n)/SiO$_2$/c-Si front side that lead to $J_{sc}$ of 42.2 mA/cm$^2$, $V_{oc}$ of 738 mV, FF of 85.2%, and a maximum power conversion efficiency of 26.6%.

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REFERENCES


SUPPORTING INFORMATION

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