Transparent silicon carbide/tunnel SiO2 passivation for c-Si solar cell front side: Enabling $J_{sc} > 42$ mA/cm² and $iV_{oc}$ of 742 mV

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Abstract

N-type microcrystalline silicon carbide ($\mu$-c-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 $\mu$-c-SiC:H(n) for c-Si solar cells with interdigitated back contacts (IBC). We demonstrate outstanding passivation quality of $\mu$-c-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 $\mu$-c-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/$\mu$-c-SiC:H(n) and 0.62 mA/cm² with MgF₂/$\mu$-c-SiC:H(n). Finally, calculations with Sentaurus TCAD simulation using MgF₂/$\mu$-c-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 \((V_{oc})\) than using SiO2 passivation3 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 bandgap6–7 of 2.4 to 3.4 eV. This high optical transparency makes it a promising window layer material,8 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 \((V_{oc})\) of up to 728 mV and saturation current densities \((J_{sc})\) 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, e.g., 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 highest short-circuit current densities \((J_{sc})\), 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 \(J_{sc}\) 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,14 42.6 mA/cm² for ISFH POLO-IBC,2 and 42.7 mA/cm² for UNSW PERL.14 All \(J_{sc}\) 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 \(J_{sc}\) 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. The derived k is zero for SiNx:H and MgF₂. The refractive index of MgF₂ is 1.4, of SiNx:H is 2.0 to 2.2, and of μc-SiC:H(n) is 2.6 to 3.0 over the wavelength range of 300 to 900 nm. Within the
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 Si\(_x\)N\(_y\)H\(_z\) are zero over the whole wavelength range. For \( \mu c\text{-SiC:H}(n) \), 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 \( \mu c\text{-SiC:H}(n) \), Si\(_x\)N\(_y\)H\(_z\), 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\(_2\)/Si\(_x\)N\(_y\)H\(_z\)/\( \mu c\text{-SiC:H}(n) \)/SiO\(_2\)/c-Si stack was calculated for different thicknesses of \( \mu c\text{-SiC:H}(n) \) (\( d_{\text{SiC}} = 0\text{-}60 \text{ nm} \)). The thickness of MgF\(_2\) was kept constant at 100 nm, and Si\(_x\)N\(_y\)H\(_z\) 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 \( (J_{\text{sim}, \text{abs}}) \) in Figure 5 that was calculated from the extinction coefficient of \( \mu c\text{-SiC:H}(n) \). We observe that \( J_{\text{sim}, \text{abs}} \) 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:

1. 108 nm MgF\(_2\)/75 nm Si\(_x\)N\(_y\)H\(_z\)/30 nm \( \mu c\text{-SiC:H}(n) \),

![FIGURE 4](image-url) Reflectance of triple-layer ARC as presented in Figure 1 with (A) simulated using OPAL2 and also (B) measured on fabricated samples. (C) SEM image of triple-layer cross section for fine adjustment of layer thicknesses [Colour figure can be viewed at wileyonlinelibrary.com]

![FIGURE 5](image-url) Optical losses of current density on front side of IBC c-Si solar cell with triple-layer ARC (see Figure 1) as a function of the \( \mu c\text{-SiC:H}(n) \) layer thickness. Presented are (A) simulated and (B) measured current loss densities rising from parasitic absorption and reflection loss. Measured current loss densities were obtained from fabricated ARC samples. To calculate the current loss due to reflection, the reflectance spectra (Figure 4) were multiplied by the AM1.5G spectra and then integrated from 300 to 990 nm that were used for integration. Parasitic absorption loss was calculated from \( k \) data of \( \mu c\text{-SiC:H}(n) \) shown in Figure 3B [Colour figure can be viewed at wileyonlinelibrary.com]
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]
comparable thickness. For a wafer thickness of 165 µm, the estimated practical limit for $i_{V_{oc}}$ is 748 mA according to Yoshikawa et al. To achieve such values close to the practical limit, Taguchi et al. claim that an ultraclean surface is needed, which was not assured for the sample preparation of this work as the HWCVD growth of $μ$-SiC:H(n) was not performed in a clean room. Compared with TOP-Con/POLO technology, the $J_0$ values of $μ$-SiC:H(n)/SiO$_2$ passivation are among the lowest $J_0$ values reported in the recent past for wet-chemically grown oxides ranging from 1.5 to 20 fA/cm$^2$. The improvement in $μ$-SiC:H(n)/SiO$_2$ passivation as compared with our former work 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 $μ$-SiC:H(n) deposition. It is important to notice that this excellent level of passivation only requires wet-chemical oxidation and HWCVD deposition of $μ$-SiC:H(n), which makes it a very simple and lean fabrication process. No further hydrogenation (through, e.g., SiNx, forming gas, Al$_2$O$_3$, and remote hydrogen plasma) and no further recrystallization at high temperatures are required. In order to understand the mechanisms for this lean passivation method, investigations are currently ongoing and will be the scope of another paper. The combination of solely wide bandgap materials gives rise to $μ$-SiC:H(n)/SiO$_2$ being a very transparent passivation.

To maximize $J_{sc}$ of the final IBC solar cell, it was important to minimize the sum of reflection and parasitic absorption losses on the front side by tuning the thickness of $μ$-SiC:H(n). According to TCAD simulations, using 30 nm of $μ$-SiC:H(n) minimizes the total optical losses of the front side to 0.47 mA/cm$^2$ for MgF$_2$/Si$_x$N$_{1-x}$:H/$μ$-SiC:H(n) and to 0.62 mA/cm$^2$ for MgF$_2$/Si$_x$C:H(n), which enable very high $J_{sc}$. For comparison, the total loss of the Si$_x$N$_{1-x}$/SiO$_2$ reference stack is 1.09 mA/cm$^2$.

Since extinction coefficients of MgF$_2$ and of Si$_x$N$_{1-x}$H are zero over the whole wavelength range, all parasitic absorption of the developed ARC takes place in $μ$-SiC:H(n) layer, which absorbs significantly for $λ$ < 520 nm. As compared with the parasitic absorption loss of 5 nm a-Si:H(0), which is approximately 1.5 mA/cm$^2$, 30 nm $μ$-SiC:H(n) absorbs 10 times less incoming sunlight (0.15 mA/cm$^2$), which shows the great potential of this layer. To further increase the transparency of the $μ$-SiC:H(n), a possible way is to increase the filament temperature during the HWCVD growth of $μ$-SiC:H(n) as it was reported before in previous studies. However, we also reported in Köhler et al. that higher filament temperatures decrease the $μ$-SiC:H(n)/SiO$_2$ passivation quality strongly. How to overcome this trade-off between transparency and passivation is currently under investigation. Additionally, the influence of the filament temperature on the refractive index needs to be studied, and possibly, the thicknesses of MgF$_2$ and $μ$-SiC:H(n) need to be readjusted. The even simpler case of MgF$_2$/SiO$_2$/c-Si, where MgF$_2$ would be evaporated on top of the SiO$_2$ tunnel oxide, is not taken into account since we found that the thin wet-chemical tunnel oxide alone cannot provide a decent passivation.

Finally, using MgF$_2$/$μ$-SiC:H(n) as ARC for IBC solar cells offers a simple and lean process flow and gives rise to the best simulated device performance of this work. It should be noticed that, although the total front losses are lowest using MgF$_2$/Si$_x$N$_{1-x}$:H/$μ$-SiC:H(n) ARC, the rear reflection losses are 2.11 mA/cm$^2$, whereas they are only 1.88 mA/cm$^2$ using MgF$_2$/$μ$-SiC:H(n) ARC. Consequently, the MgF$_2$/ $μ$-SiC:H(n) ARC leads to slightly higher $J_{sc}$ and $η$ in the simulated devices. On low-cost wafer, it gives rise to an efficiency of 25.2% and a $J_{sc}$ of 42.0 mA/cm$^2$. This is in the range of tunnel-junction IBC solar cells, which achieved a certified $η$ of 25.0% and $J_{sc}$ of 41.7 mA/cm$^2$ very recently and which also follow the idea of simple fabrication process. On high-quality c-Si wafer, with $τ_{bulk} = 12$ ms, we calculated 26.6% for $η$, 42.24 mA/cm$^2$ for $J_{sc}$, 738 mV for $V_{oc}$, and 85.2% for $FF$. As compared, the best IBC solar cell fabricated by Kaneka gave rise to a certified $η$ of 26.7%, 42.65 mA/cm$^2$ for $J_{sc}$, 738 mV for $V_{oc}$, and 84.9% for $FF$. The main difference arises from 0.41 mA/cm$^2$ lower $J_{sc}$ for the MgF$_2$/$μ$-SiC:H(n) stack, which might be increased by enhanced light trapping, further minimization of parasitic absorption in the $μ$-SiC:H(n) layer, and readjusting the thicknesses of MgF$_2$ and $μ$-SiC:H(n).

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 $μ$-SiC:H(n) on top. Excellent passivation properties with a reproducible $i_{V_{oc}}$ of 742 mV and $J_0$ of 3.6 fA/cm$^2$ were achieved directly after the HWCVD deposition of $μ$-SiC:H(n), without any further treatments like recrystallization or hydrogenation. Because of its high transparency and its suitable refractive index, we developed MgF$_2$/$μ$-SiC:H(n) and MgF$_2$/Si$_x$N$_{1-x}$:H/$μ$-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$_2$/$μ$-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%.

ACKNOWLEDGEMENTS

This project has received funding from the European Union’s Horizon2020 Program for research, technological development and demonstration under grant agreement no. 727523. A. Zamchiy would especially acknowledge the financial support from the German Academic Exchange Service (DAAD) and the Ministry of Education and Science of the Russian Federation (”Mikhail Lomonosov” program, project NM3705).

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SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section at the end of this article.

How to cite this article: Pomaska M, Köhler M, Procel P, Moya P, et al. Transparent silicon carbide/tunnel SiO2 passivation for c-Si solar cell front side: Enabling Jsc > 42 mA/cm² and IV curve of 742 mV. Prog Photovolt Res Appl. 2020;1–7. https://doi.org/10.1002/pip.3244