

PASSIVATION AND MICROSTRUCTURE OF DUAL INTRINSIC a-Si:H LAYERS FOR SHJ SOLAR CELLS

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ABSTRACT: We demonstrate a high passivation quality of dual a-Si:H(i) layers with excellent implied open circuit voltage values and a beneficial influence by an intermediate H₂ plasma treatment made with an industrial inline PECVD tool from Meyer Burger Germany with radio frequency plasma sources (MAiA tool). Furthermore, the correlation between the gas flow ratio of hydrogen to silane during PECV deposition and the microstructure of the a-Si:H(i) layers represented by the relative bonding density of monohydrides (Si-H) and dihydrides (Si-H₂) obtained by ATR-FTIR analysis is shown. Also the positive impact of an intermediate H₂ plasma treatment is illustrated. Finally the resulting passivation quality reached by the use of dual a-Si:H(i) layers is depicted, which enables a significant improvement of the implied open-circuit voltage compared to the single layers, especially in the case of a-Si:H(i/p) layer stacks.

Keywords: Silicon Heterojunction, a-Si:H, Passivation, Microstructure

1 INTRODUCTION AND MOTIVATION

Silicon Heterojunction (SHJ) solar cells represent a key technology to approach very high conversion efficiencies close to the theoretical limit of silicon solar cells [1]. The main advantages of SHJ solar cells are a lean production chain with low temperature processes and carrier selective hetero-structures for excellent passivation. To reach this passivation quality it is crucial to reduce the losses caused by surface recombination at the interface of the crystalline silicon (c-Si) substrate via hydrogenated amorphous silicon (a-Si:H) layers. Both-side contacted SHJ solar cells featuring amorphous thin-film layer stacks enable high conversion efficiencies up to 26.6% [2]. To achieve such high efficiencies not only the quality of the a-Si:H layers and the c-Si surface structure must be carefully optimized, but also different features as the front grid electrode and the transparent conductive oxide (TCO) play a major role. Aiming to reduce the cost of owner-ship (COO) an increased throughput is required which can be realized within an inline plasma enhanced chemical vapour deposition (PECVD) process. In this work we use an industrial MAiA PECVD tool from Meyer Burger Germany (MBG), which is equipped with radio frequency (RF) plasma sources to develop depositions of intrinsic and doped a-Si:H layers.

As mentioned previously, passivation of the c-Si interface is crucial to reach very high conversion efficiencies. Therefore two essential requirements have to be fulfilled by the intrinsic a-Si:H layer (a-Si:H(i)) to improve implied open-circuit voltage iV_{OC} : (1) preventing epitaxial growth and (2) saturating dangling bonds at the c-Si surface and within the a-Si:H layers. An innovative approach is the deposition of dual-/multi a-Si:H(i) layers, consisting of a soft interfacial buffer layer with low hydrogen (H₂) content (named i1) to prevent epitaxial growth and a second layer with high hydrogen dilution (named i2) to enhance passivation by saturating dangling bonds retrospectively within the i1-layer and increase the film density, featuring less micro voids [3,4,5]. Furthermore an impact of an additional H₂ plasma treatment on the passivation quality [6,7,8] and also on the microstructure was observed, either after deposition of a-Si:H(i) layer or as an intermediate step between i1 and i2 [9]. In this work we investigated the microstructure of a-Si:H layers produced in an industrial

inline PECVD tool and proved that in the case of a-Si:H(i/p) layer stacks the dual layer approach leads to significantly higher passivation quality compared to the a-Si:H(i/p) stack with a single intrinsic layer.

2 EXPERIMENTAL SETUP

2.1 Sample structure

The investigated sample structure consists of both planar (shiny etched) and alkaline textured n-type float zone (FZ)-Si wafers with an initial thickness of 200 μm, a resistivity of 1 Ω*cm and (100)-orientation. Figure 1 depicts the fabricated sample structures. Both sample types, with a-Si:H(i) deposited only on one side (Fig. 1a) as well as symmetrically deposited samples with either a 10 nm thick a-Si:H(i) on both sides (Fig. 1b) or with a stack of i1- and i2-layers (each 5 nm thick, Fig. 1c) were produced, where a-Si:H deposition was performed using mixtures of SiH₄ and H₂. The one-sided coated planar samples were used to determine layer thickness d via spectroscopic ellipsometry (SE); with a Woollam M-2000 Ellipsometer as well as the textured ones to determine the microstructure factor R^* via Attenuated Total Reflection Fourier-Transform Infrared Spectroscopy (ATR-FTIR) by Bruker VERTEX 80v. The symmetrical samples (Fig. 1b,c) were used to investigate the implied open circuit voltage (iV_{OC}) to evaluate the passivation quality of the different layer structures by quasi steady-state photoconductance (QSSPC) measurement with a WCT-120 tool from Sinton Instruments in the center of the wafer. The samples were prepared on both planar and textured surfaces, whereas they were prepared in the same PECVD process, which means that due to the larger surface area of the textured samples they are thinner by a factor of ~1.4.

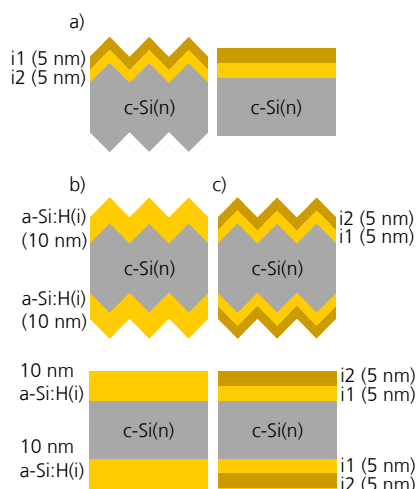


Figure 1: Schematic illustration of the samples (textured and planar) used to investigate the a-Si:H(i) single and dual layers; (a) SE/ATR-FTIR samples, (b,c) QSSPC samples.

2.2 Investigated layer systems

Fig. 2 shows the process sequences where different a-Si:H(i) single and dual layers and a subsequent or intermediate H₂ plasma treatment were investigated. Group 0 represents the previous reference process which consists of a single layer with a ratio of hydrogen gas flow ϕ_{H_2} to silane gas flow ϕ_{SiH_4} of $R_{gas} = \phi_{H_2}/\phi_{SiH_4} = 4.5$ during the process. Group 1 represents a single layer made out of a pure SiH₄ plasma and group 2 features the same layer as group 1 but with a subsequent H₂ plasma treatment. The samples in group 3 are deposited with a dual a-Si:H layer consisting of group 1 as i1- and group 0 as i2-layer. Finally group 4 to 7 shows dual a-Si:H layers where the i1-layer equals to that layer of group 2 and the i2-layer includes a variation of the gas flow ratio during i2-layer deposition $R_{gas,i2}$ where we increased the H₂ gas flow ϕ_{H_2} from group 4 to 7 leading to higher $R_{gas,i2}$ and also increased total gas flow. Furthermore symmetrical lifetime samples with a-Si:H(i/p) layer stacks with single as well as dual a-Si:H(i) layers and a variation of the B₂H₆ doping gas flow during PECVD of the a-Si:H(p)-layer were fabricated (group 8-12) where the thickness of the a-Si:H(p) layer thickness was kept constant at 10 nm for all groups.

Layer-by-layer analysis			
Group	Interfacial layer i1	Capping layer i2	a-Si:H(p)
0	SiH ₄ + H ₂ , $R_{gas} = 4.5$		-
1	SiH ₄	-	-
2	SiH ₄ + H ₂ plasma treatment	-	-
3	SiH ₄	SiH ₄ + H ₂ , $R_{gas} = 4.5$	-
4 to 7	SiH ₄ + H ₂ plasma treatment	SiH ₄ + H ₂ , $R_{gas} = 4.5/20/25/40$	-
8-10	SiH ₄ + H ₂ , $R_{gas} = 4.5$		p, p ⁺ , p ⁺⁺
11-12	SiH ₄ + H ₂ plasma treatment	SiH ₄ + H ₂ , $R_{gas} = 20$	p, p ⁺

Figure 2: Process sequences of a-Si:H(i) single vs. dual layers and influence of H₂ plasma treatment performed on all sample structures shown in Fig. 1

To investigate the passivation quality of the a-Si:H(i) single and dual layers at first ellipsometry samples (Fig. 1a) were deposited to adjust the thickness of the layers for the lifetime samples (Fig. 1b) to 10 nm or to 5 nm for i1- and 5 nm for the i2-layer (Fig.1 c).

3 A-SI:H(I) SINGLE VS. DUAL LAYERS

3.1 Passivation properties

Fig. 3 depicts the iV_{OC} values on planar surfaces. The reference process (group 0) leads to very low iV_{OC} values of around 640 mV and since the SE measurement does not provide typical a-Si:H layer properties, we conclude that epitaxial/partially crystalline growth occurs at the c-Si surface. Very high passivation quality (up to iV_{OC} of 747 mV) was reached with a pure SiH₄ plasma grown layer at the interface (group 1), whereas a subsequent H₂ plasma treatment only leads to a minor improvement (group 2). The addition of a i2-layer in group 3 leads to a drop in passivation quality down to around 700 mV compared to group 1, probably due to partially crystalline growth at the interface between i1- and i2-layer and/or less hydrogen within the layer to saturate the dangling bonds. We reached excellent passivation quality with iV_{OC} values above 740 mV for group 4 which is a combination of group 2 (i1-layer) and group 0 (i2-layer). The subsequent H₂ plasma treatment

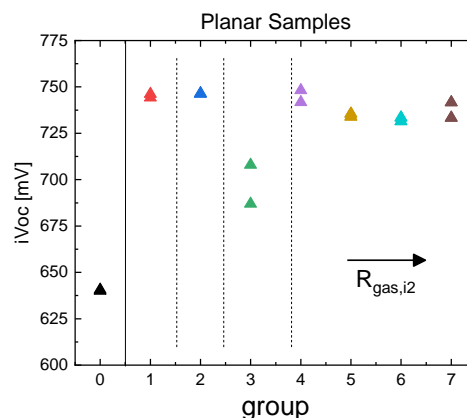


Figure 3: Implied V_{OC} for a-Si:H(i) single vs. dual a-Si:H(i) layers for different process sequences on planar samples, whereas group 4 to 7 show an increase of R_{gas} during i2 layer deposition.

seems to increase the structural disorder within the layer and at the interface and therefore effectively avoids partially crystalline growth which agrees with the observed improvement of iV_{OC} from group 3 to 4. Group 5 to 7 represent an increase of $R_{gas,i2}$ during i2-layer deposition which leads to a minor decrease of iV_{OC} , but still remains at values above 730 mV. One hypothesis for the decrease is a partially crystalline growth respectively dissociation of weak bonds by etching in the growing a-Si network which creates voids and/or less hydrogen within the layer to saturate the dangling bonds. Nevertheless, our results show the potential of the dual a-Si:H(i) layer approach and prove the beneficial effect of an intermediate H_2 plasma treatment.

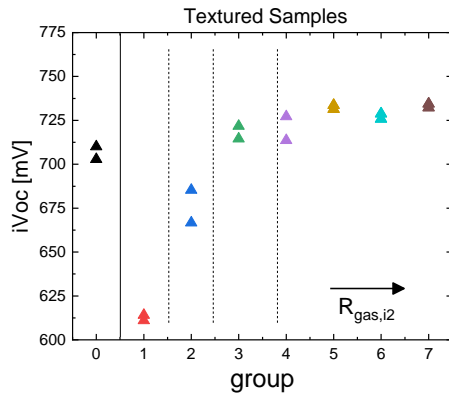


Figure 4: Implied V_{OC} for a-Si:H(i) single vs. dual a-Si:H(i) layers for different process sequences on textured samples, whereas group 4 to 7 show an increase of R_{gas} during i2-layer deposition.

Fig. 4 depicts the results on textured samples. The SiH_4+H_2 based process (group 0) leads to moderate iV_{OC} values above 700 mV. The very low iV_{OC} of a single a-Si:H(i) layer deposited with a pure SiH_4 plasma (group 1) presumably can be explained by an insufficient coverage of pyramids due to the thinner layer thickness on textured surfaces and the very low gas volume by only using SiH_4 as a process gas. Group 2 shows a beneficial effect by a H_2 plasma treatment on the layer made out of a pure SiH_4 plasma process. Group 3 and 4 obviously gain from the dual a-Si:H(i) layer approach and reach iV_{OC} values of around 720 mV which is quite remarkable for these initial experiments. We attribute the increase in iV_{OC} to the fact, that a sharp/abrupt interface between a-Si and c-Si is required for preventing epitaxial growth which is given by a layer with a higher disorder within the structure which is the fact in case of a less dense layer. The layers with lower density (group 1) suffer from inferior passivation quality due to less hydrogen content. Therefore we treat the surface with hydrogen plasma (group 2) to potentially increase the hydrogen content retrospectively within i1 and prepare the surface of i1 by increasing the disorder to also avoid epitaxial growth of the i2. Finally a second a-Si:H layer (i2 from group 5) reduces micro-voids within the a-Si:H film to increase the film density and also subsequently improve the passivation quality of the i1-layer.

In summary, Group 4 represents a feasible process for both planar and textured surfaces. This process enables iV_{OC} up to 747 mV on planar and around 720 mV on textured surfaces. By further increasing $R_{gas,i2}$ during

i2-layer deposition (group 4 to 7), iV_{OC} increases up to 730 mV.

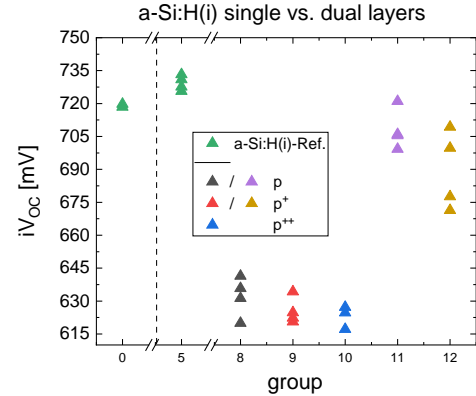


Figure 5: Implied V_{OC} for a-Si:H(i/p) layer stacks with a-Si:H(i) single and dual layers on textured samples with a variation of B_2H_6 gas flow during PECVD.

Fig. 5 shows the iV_{OC} values of a-Si:H(i/p) layer stacks with a-Si:H(i) single and dual layers on textured samples. Group 0 depicts the iV_{OC} value of only the a-Si:H(i) layer ($iV_{OC} \sim 720$ mV) and group 8-10 with a-Si:H(p) layer on top with an increase of B_2H_6 gas flow. Deposition of a-Si:H(p) on top of the single a-Si:H layer results in a significant decrease in iV_{OC} (below 640 mV). Group 5 shows the iV_{OC} (> 730 mV) of only the dual a-Si:H(i) layer and 11 and 12 presents the decrease of iV_{OC} by deposition of a-Si:H(p) layer on top with increasing B_2H_6 gas flow. As one can see in the case of dual a-Si:H layers the deterioration of iV_{OC} is much less pronounced compared to the a-Si:H(i) single layers.

3.1 Microstructure factor R^*

For each variation shown in the previous chapter, we also performed ATR-FTIR measurements to investigate if we can correlate the deposition parameters, especially R_{gas} to the microstructure of the a-Si:H layers and also the passivation properties. Fig. 6 shows the ATR-FTIR spectra evaluated with regard to the Si-H and Si-H₂ bonds. These were now analysed regarding the microstructure factor R^* , which is defined as the ratio of the integrated area under the fitted curve of the signal of dihydrides (Si-H₂) relative to the sum of the integrated area under the fitted curve of the signal of clustered monohydrides (Si-H) and dihydrides (Si-H₂) bonding species:

$$R^* = \frac{I_{Si-H_2}}{I_{Si-H_2} + I_{Si-H}}$$

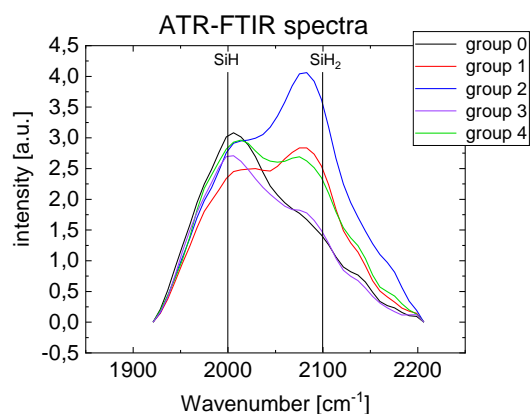


Figure 6: ATR-FTIR spectra evaluated with regard to Si-H and Si-H₂ bonds expected at 2000 cm⁻¹ and 2100 cm⁻¹, respectively, of the different process sequences shown in Fig. 2.

Low R^* means that the dominant bond is Si-H (black curve in Fig. 6) which implies a dense a-Si:H(i) layer, while a high R^* stands for Si-H₂ as the dominant bond which represents less dense a-Si:H(i) layers (blue curve in Fig. 6).

Fig. 7 depicts the R^* -values for the different process sequences whereas the groups are the same as in Fig. 3 and 4. Group 0 has a very low R^* and as one can see (black curve in Fig. 6) the Si-H peak dominates this spectrum which means that this a-Si:H layer is very dense and has a low concentration of hydrogen. That leads to the inferior passivation quality and epitaxy at the c-Si surface as shown before. Group 1, the pure SiH₄ plasma (no H₂ gas flow during process), leads to an increase of the Si-H₂ peak (red curve in Fig. 6) which leads to an increased hydrogen content within the layer. Fig. 7 shows an increase in R^* which corresponds to an increase in disorder (decreased density within layer). That correlates to the very high iV_{OC} on planar surfaces as it creates an abrupt interface and therefore effectively avoids epitaxy. Group 2 (pure SiH₄ plasma and subsequent H₂ plasma treatment) has the highest value of R^* and hence the highest Si-H₂ bond peak (blue curve in Fig. 6). This shows a distinct influence of the H₂ plasma treatment which significantly increases the hydrogen content within the layer. The treatment leads to an increased disorder which avoids epitaxy and leads to a high passivation quality on planar surfaces. Also the textured samples benefit from a secondary passivation due to hydrogen plasma (increasing the hydrogen content within the layer), but still end up with an insufficient iV_{OC} . Group 3 (dual layer consisting of group 1 as i1 and group 0 as i2) leads to a lower R^* than group 1, and the Si-H peak is dominant which is similar concerning the resulting layer properties to group 0. Since the utilized method does not provide a spatially resolved measurement, it is very likely that we measure some sort of integrated signal of both layers of group 3 and 4 and therefore end up with an integrated R^* of both layers. Nevertheless one can see an increase in passivation quality for this layer stack on textured surfaces, which confirms the improvements of passivation quality by the dual a-Si:H(i) layer approach. The planar samples within group 3 probably suffer from partially crystalline growth (same effect as in group 0, either at the c-Si surface and/or at the interface of i1 and i2) and/or less hydrogen within the layer to saturate the

dangling bonds, which leads to an inferior passivation quality. Group 4, which is a combination of group 2 as i1 and group 0 as i2 is characterized by an R^* value which lies between that of group 2 and group 0. Again this leads to the conclusion of an integrated signal of both layers. At the end this combination is the most promising with excellent passivation quality on both surfaces which confirms that the a-Si/c-Si interface design is very important and can be successfully implemented by the approach of dual a-Si:H(i) layers. The dual a-Si:H layer stack should therefore have the following properties: i1 requires a low H₂ gas flow (low R_{gas}) to have a high hydrogen content within the layer which leads to high R^* . That in turn leads to a less dense, disordered layer that avoids epitaxial growth at the c-Si surface and therefore a sharp/abrupt interface. Subsequent H₂ plasma treatment further increases this disorder and potentially also increases hydrogen within the i1-layer to saturate dangling bonds. Afterwards the i2-layer requires a high H₂ gas flow (high R_{gas}) to have a low concentration of hydrogen within the layer which leads to low R^* that creates a denser layer to reduce micro-voids and increase the layer density and subsequently improve passivation of the i1-layer.

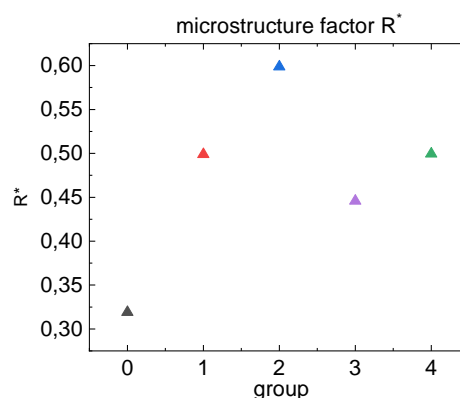


Figure 7: R^* values calculated from the spectra shown in Fig. 6 for the different process sequences shown in Fig. 2.

4 CONCLUSION

We investigated different process sequences regarding the microstructure by analysing the microstructure factor R^* and were able to correlate that to the passivation properties (represented by the iV_{OC}). We developed a feasible process for both planar and textured surfaces which leads to $iV_{OC} > 740$ mV on planar and up to 735 mV on textured surfaces. Furthermore a beneficial effect of an intermediate H₂ plasma treatment has been demonstrated. In addition we were able to work out a correlation between the gas flow ratio R_{gas} and the microstructural factor R^* of the resulting single and dual a-Si:H layers.

It could be demonstrated that the a-Si/c-Si interface design is very important and can be successfully implemented by the approach of dual a-Si:H(i) layers to improve the passivation quality especially in the case of a-Si:H(i/p) layer stacks.

5 ACKNOWLEDGEMENTS

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