






# Controlling Diffusion in Poly-Si Tunneling Junctions for Monolithic Perovskite/Silicon Tandem Solar Cells

Christoph Luderer , Michaela Penn, Christian Reichel, Frank Feldmann , Jan Christoph Goldschmidt , Susanne Richter, Angelika Hähnel , Volker Naumann , Martin Bivour, and Martin Hermle

**Abstract**—The performance of a low-resistive  $p^+/n^+$  poly-Si tunneling junction (SiTJ) based on a tunnel oxide passivating contact in dependence on the thermal budget of the applied post-deposition treatment is studied. We present two approaches to reduce the performance limiting parasitic dopant interdiffusion and, thus, the contact resistivity, without impairing the passivation quality. Both, carbon-alloying of poly-Si layers and the application of diffusion blocking interlayers are effective means to maintain a low contact resistivity of  $\sim 24 \text{ m}\Omega\text{cm}^2$  at high thermal process temperatures of up to  $950^\circ\text{C}$ . Those low values are obtained using either a standard furnace anneal or a rapid thermal process (RTP). We report on promising results toward a lean process sequence using only one single fast thermal treatment (RTP-only). As a main result, the flexibility for engineering and fabrication of our SiTJ was markedly improved, eventually facilitating industrially feasible perovskite/silicon tandem solar cells. One aspect being higher post-deposition temperatures needed for, e.g., bottom cell rear side contact formation and the first layers of the perovskite to cell.

**Index Terms**—Contact resistivity, passivating contact, perovskite-silicon tandem, solar cells, tunneling junction.

## I. INTRODUCTION

WITH the recent world record efficiency of 29.5% for a perovskite/silicon tandem [1] exceeding the theoretical efficiency limit of 29.4% for a silicon (Si) single junction [2], tandem solar cells are getting more and more attention from the photovoltaic community. The combination of a perovskite cell on top of a crystalline-Si (c-Si) bottom cell is thereby especially attractive, as they promise high efficiency at affordable costs [3]–[5]. For straightforward module and system integration, the monolithic two-terminal tandem configuration is preferred.

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Such a configuration requires low-ohmic and transparent interconnection of both subcells. Transparent conductive oxides are widely used to serve that purpose [6]–[8]. An alternative are Si-based tunneling junctions (SiTJs), as first demonstrated in a perovskite/Si tandem cell by Mailoa *et al.* [9], which have the benefit of better refractive index matching between the subcells and thus reducing reflection losses [10]. Additionally, they have the potential to be directly integrated in the processing of the bottom cell's passivating contact [11]–[15]. Compared to silicon heterojunction (SHJ)-based SiTJ, poly-Si-based passivating TJs [11], [14] have the benefit of higher thermal stability, making them compatible with the mainstream Si solar cell structure, i.e., the passivated emitter and rear cell (PERC) technology [16] [see Fig. 1(c)]. Further, a temperature stable bottom cell and SiTJ might be preferable for future application, as lead-free perovskite absorbers are supposed to need annealing temperatures exceeding the stability of SHJ bottom cells [17].

Previously, we presented a low-resistive and passivating SiTJ based on a poly-Si( $p^+$ )/poly-Si( $n^+$ )/ $\text{SiO}_x$ /c-Si stack [11]. It was shown that its performance is strongly influenced by dopant interdiffusion during post-deposition thermal treatments. Based on this, in this work, the diffusion behavior for different thermal budgets will be studied. Further, two approaches to reduce parasitic interdiffusion will be presented. Finally, the microstructure of the poly-SiTJ is briefly discussed.

## II. EXPERIMENTAL

SiTJ structures were fabricated with two different process routes, as depicted in Fig. 1(a). For both process sequences,  $200 \mu\text{m}$  thick planar  $1 \Omega\text{cm}$  n-type FZ silicon wafers were used as a substrate. After RCA cleaning, a  $\sim 1.2 \text{ nm}$  thin tunnel oxide layer was thermally grown in a furnace at  $600^\circ\text{C}$  for 10 min. Subsequently, 20–50 nm thick phosphorus (P)-doped Si layers were deposited on both sides via plasma-enhanced chemical vapor deposition (PECVD), yielding symmetrical a-Si:H( $n^+$ )/ $\text{SiO}_x$ /c-Si( $n$ )/ $\text{SiO}_x$ /a-Si:H( $n^+$ ) structures. For route “FA+RTP,” these structures were exposed to a tube furnace anneal (FA) at  $900^\circ\text{C}$  for 10 min to “activate” TOPCon (i.e., poly-crystallization of the phosphorus-doped a-Si:H layer, diffusion of dopants into the absorber and modification of the  $\text{SiO}_x$ /Si interface). This FA was omitted for samples in route “RTP-only.” Then, 20 nm thick boron (B)-doped PECVD a-Si:H layers were deposited on one side. For some samples, methane gas was introduced in the reactor chamber during PECVD, yielding carbon (C)-alloyed

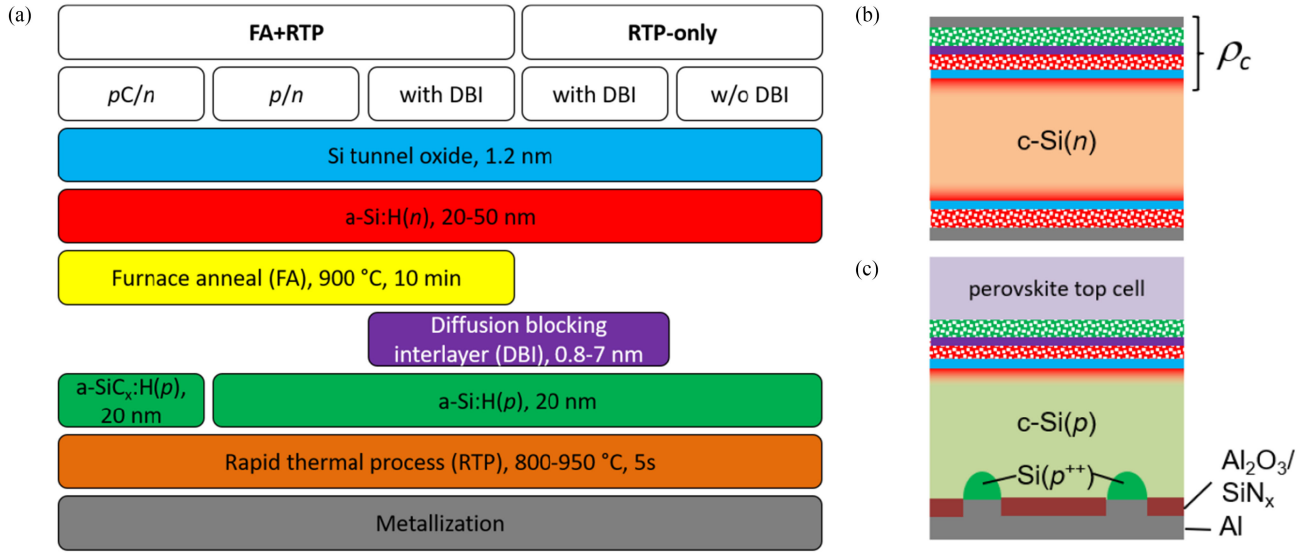


Fig. 1. (a) Process sequences for fabricated SiTJ with (“FA + RTP”) and without FA (“RTP-only”). (b) Sketch of the sample structure for dark  $J$ - $V$  measurements. (c) Proposed bottom cell structure with PERC rear side, a front side poly-Si passivating contact and a  $p^+/n^+$  poly-SiTJ as subcell interconnection in monolithic perovskite/Si tandem solar cells.

a-SiC<sub>x</sub>:H(p<sup>+</sup>). SiTJ comprising such C-alloyed B-doped layers are referred to as pC/n SiTJ. For some other samples, a potential dopant diffusion blocking interlayer (DBI) was deposited directly before a-Si:H(p<sup>+</sup>) deposition. Several DBIs were tested, including SiO<sub>x</sub> grown either thermally (“TO”), wet-chemically (“HNO<sub>3</sub>”) or via atomic layer deposition (ALD, “SiO<sub>x1</sub>” and “SiO<sub>x2</sub>”), further PECVD SiC<sub>x</sub> and ALD SiN<sub>x</sub>. Finally, the samples were exposed to a rapid thermal annealing process (RTP) with peak plateau temperatures  $T_{RTP}$  in the range of 800–950 °C and a peak time of 5 s each. To assess the contact resistivity ( $\rho_c$ ) of the SiTJ, a stack of Ti/Pd/Ag was thermally evaporated on both sides of the samples, which were cut into square  $0.5 \times 0.5$  cm<sup>2</sup> pieces using a dicing saw. Depicted  $\rho_c$  values throughout the text represent the combined junction resistance of both the SiTJ and the tunnel oxide passivated front contact (TOPCon). Bulk and rear contact contributions were subtracted using equally processed symmetric poly-Si(n<sup>+</sup>) reference samples, where the B-doped Si layer was omitted. The implied open-circuit voltage ( $iV_{oc}$ ) at 1 sun illumination was measured after a hydrogenation step for selected samples as a figure of merit for the passivation quality. Dopant depth profiles were measured with the electrochemical capacitance-voltage (ECV) method and time of flight secondary-ion mass spectroscopy (ToF-SIMS) using an IONTOF TOF.SIMS 5. The Si thin film microstructure was recorded using transmission electron microscopy (TEM) in an image-corrected FEI TITAN3 G2 60-300 with 300 kV electron beam energy.

### III. RESULTS

#### A. Standard p/n SiTJ

Dopant depth profiles of regular p/n SiTJs using the FA+RTP route, as measured with ToF-SIMS, for different post-deposition thermal treatments are shown in Fig. 2. Without any post-deposition thermal treatment (neither FA nor RTP), a high

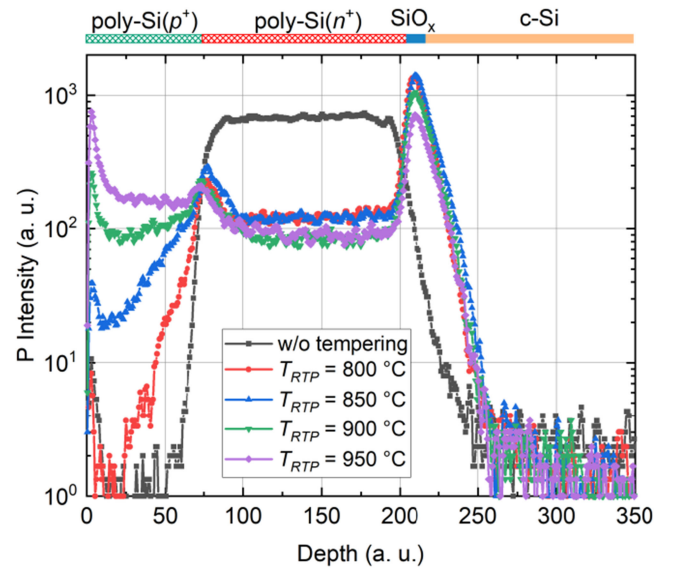


Fig. 2. Dopant depth profiles, as measured with ToF-SIMS, for different post-deposition thermal treatments. The influence of  $T_{RTP}$  on the P depth profile is shown.

and homogenous phosphorous (P) concentration was observed within a-Si:H(n<sup>+</sup>) which abruptly decreased to a very low level within a-Si:H(p<sup>+</sup>) and c-Si. The asymmetry in the profile with a slightly lower slope for the tail at the a-Si:H(n<sup>+</sup>)/SiO<sub>x</sub>/c-Si interface can be explained by P atoms driven due to the sputtering process during the measurement.

The diffusion of P into the absorber at the poly-Si(n<sup>+</sup>)/SiO<sub>x</sub>/c-Si(n) interface, which supports the surface passivation [18], was defined by the FA and hardly changed by the RTP. Within c-Si, the P profiles were very similar independent of  $T_{RTP}$ .

The P intensity in the poly-Si(p<sup>+</sup>) layer was increased significantly with increasing  $T_{RTP}$ . The P plateau within poly-Si(n<sup>+</sup>)

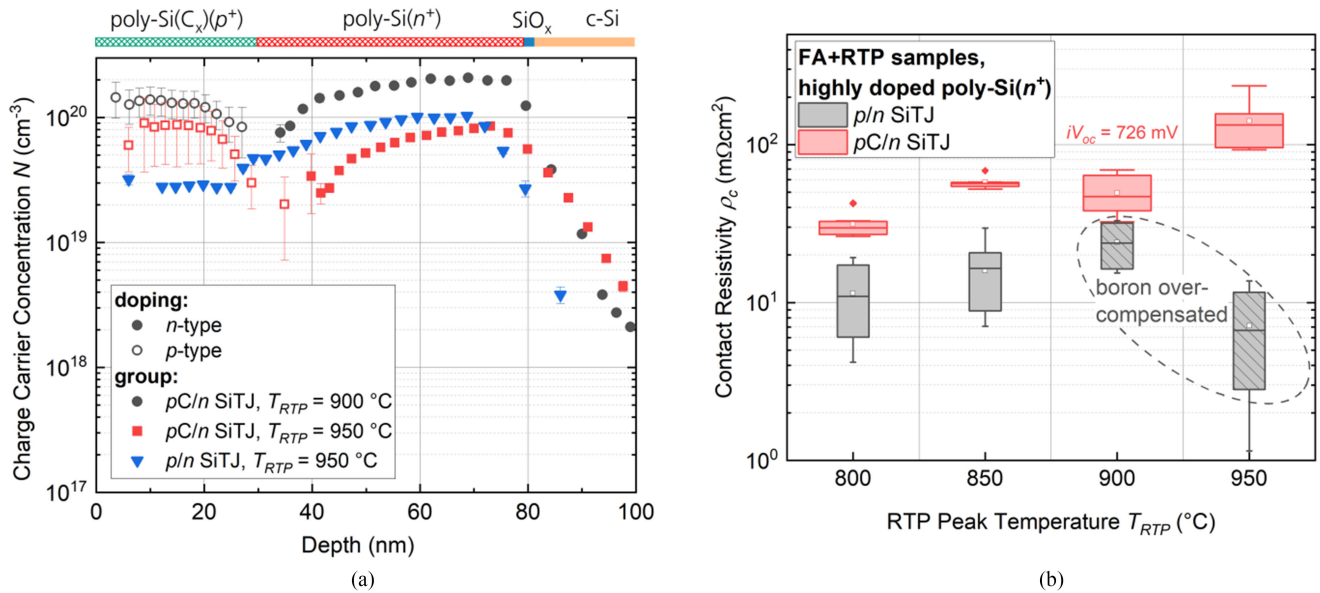


Fig. 3. (a) Active dopant concentration, as measured with ECV, of SiTJ comprising poly-Si(p<sup>+</sup>) with and without incorporated C. (b)  $\rho_c$  in dependence of  $T_{RTP}$  for p/n and pC/n SiTJ.

was decreased accordingly with increasing  $T_{RTP}$ . Apparently, P diffused into the poly-Si(p<sup>+</sup>) region during the RTP with the strength of diffusion determined by the applied thermal budget. Similarly, boron (B) diffusion from the poly-Si(p<sup>+</sup>) into the n<sup>+</sup>-region was enhanced at higher thermal budget (not shown). At  $T_{RTP} = 900$  °C, the P concentration was similar in both p-type and n-type poly-Si, and at  $T_{RTP} = 950$  °C, the P concentration was even higher in poly-Si(p<sup>+</sup>) compared to poly-Si(n<sup>+</sup>).

Prominent is the peak at the position of the thermally grown SiO<sub>x</sub> at the poly-Si/c-Si interface. It is known that SiO<sub>x</sub> is a diffusion barrier for P and that P piles up at such oxides [19], [20], which was also previously observed for TOPCon structures [18], [21]. However, quantitative analysis of the peak at the poly-Si/SiO<sub>x</sub> interface is difficult due to the so-called SIMS matrix effect, which describes the enhancement of ion yield resulting from the presence of oxygen or cesium [22], [23]. The increase of the P signal toward the poly-Si/air interface probably can be attributed to this effect since the poly-Si surface was oxidized during the RTP. More importantly, a local maximum of the P signal was observed at the position of the SiTJ. This can be explained by a thin native SiO<sub>x</sub> present at this interface, despite an HF treatment before a-Si:H(p<sup>+</sup>) deposition. The thin native oxide present at the SiTJ obviously could not provide sufficient dopant diffusion blocking, although a diffusion blocking behavior of the native SiO<sub>x</sub> was observed to some extent by comparing SiTJ deposited with and without vacuum break (not shown).

### B. Carbon-Alloyed SiTJ

Fig. 3(a) shows the active dopant concentration of a pC/n SiTJ with a carbon (C) content of less than 15 at% in the p<sup>+</sup>-region compared to a regular p/n SiTJ. Both SiTJs comprised a heavily P-doped layer. As previously discussed in [11], at  $T_{RTP} = 950$  °C

B was completely overcompensated by P in the p<sup>+</sup>-region of the p/n SiTJ and a fairly high electron concentration of  $N > 2.0 \times 10^{19}$  cm<sup>-3</sup> was measured throughout both poly-Si layers (blue data). Very similar results were obtained for  $T_{RTP} = 900$  °C (not shown). Please note that introducing C into the poly-SiC<sub>x</sub>(p<sup>+</sup>) leads to uncertainties regarding the absolute  $N$  values in the p<sup>+</sup>-region measured with ECV [24]. Nevertheless, it can be stated that C-alloying prevented overcompensation, as p-type doping was measured throughout the whole p<sup>+</sup>-region for both  $T_{RTP} = 900$  °C (black data) and 950 °C (red data). From Fig. 3(a), it cannot be concluded how C influenced B or P diffusion specifically. In [25], it was reported that P diffuses in poly-Si predominantly along grain boundaries whereas for B both diffusion along grain boundaries and through crystal grains is important. Since C is known to hamper the self-interstitial diffusion mechanism in Si crystals [26], especially B diffusion might be blocked in C-alloyed poly-Si. Another explanation, why C-alloying prevented overcompensation of B in Fig. 3(a) might be segregation of B to SiC at the SiC/Si interface [27]. Why C-alloying prevented overcompensation of B in Fig. 3(a). However, this cannot explain, that a similar effect was observed when the poly-Si(n<sup>+</sup>) was alloyed with C instead of the poly-Si(p<sup>+</sup>) (not shown).

Comparing  $\rho_c$  of the p/n and the pC/n SiTJ in Fig. 3(b), a higher  $\rho_c$  was observed for the pC/n SiTJ in the range  $T_{RTP} = 800$ –950 °C. The crystalline fraction, obtained by fitting spectroscopic ellipsometry data with a model assuming a mixture of poly-Si, a-Si:H and voids, and therefore also the doping efficiency was decreased considerably in poly-SiC<sub>x</sub> with increasing C content (not shown). Consequently, a lower active dopant concentration  $N$  at the p<sup>+</sup>/n<sup>+</sup> poly-Si interface and, thus, a broadened depletion width can be assumed. Hence, at  $T_{RTP} = 800/850$  °C, the higher resistance of the pC/n SiTJ can most likely be attributed to less efficient tunneling as a result of



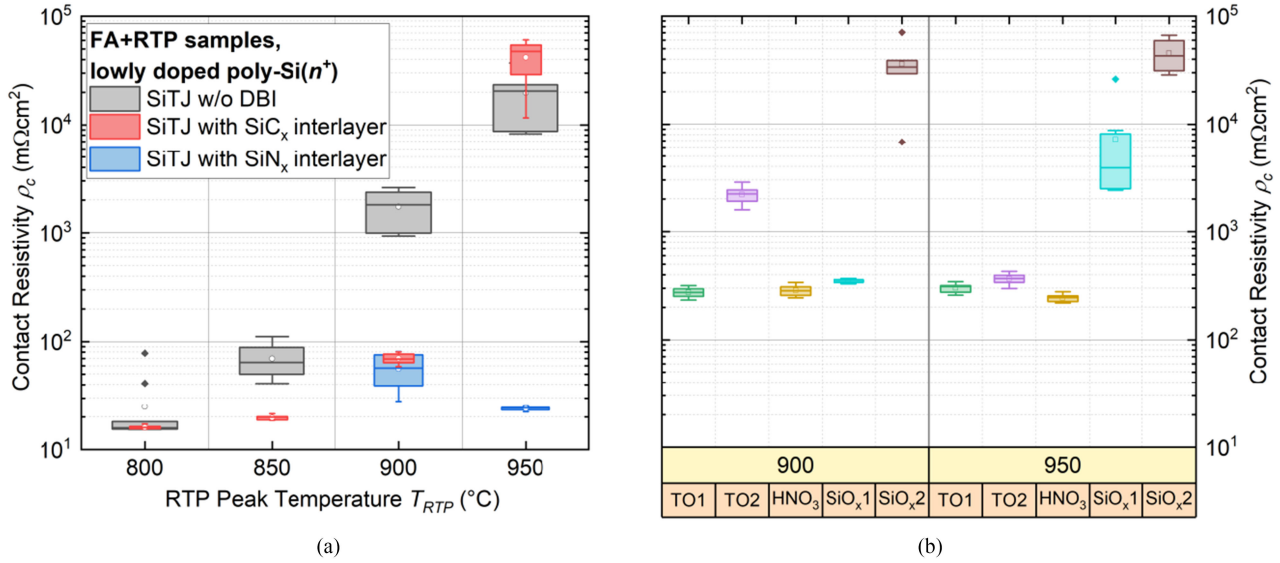


Fig. 4. Resistance in dependence of  $T_{RTP}$  for SiTJs comprising different DBIs. (a)  $\rho_c$  of FA+RTP SiTJ without DBI as reference and SiTJs with SiN $_x$  or SiC $_x$  DBI. (b)  $\rho_c$  of FA+RTP SiTJs with different SiO $_x$  DBIs.

a broadened depletion width [28]–[30]. Further, a higher “bulk” resistivity of the poly-SiC $_x$  layer itself is expected due to a lower crystalline fraction and smaller crystal grains as a result of C-alloying. At  $T_{RTP} = 900$  °C and higher temperatures, the p/n structure without C was not a tunneling junction anymore, as B was completely overcompensated by P [11], and the comparison of  $\rho_c$  is obsolete. The pC/n SiTJ, however, showed low resistance and good passivation with  $\rho_c = 47$  m $\Omega$ cm $^2$  and  $iV_{oc} = 726$  mV at  $T_{RTP} = 900$  °C. Thus, it is possible to hamper interdiffusion at the poly-SiTJ by C-alloying, thereby increasing the thermal stability of the poly-SiTJ. Another positive effect of C-alloyed poly-SiC $_x$  regarding tandem application is the increased sheet resistance (not shown), which might be beneficial to impair the connection of shunt paths in a tandem device [31]–[33] and to ease up-scaling [12], [34].

### C. Diffusion Blocking Interlayer

To show the potential as dopant DBI,  $\rho_c$  of several test structures comprising different interlayers at the SiTJ is plotted against  $T_{RTP}$  in Fig. 4(a) and (b). The regular p/n SiTJ without interlayer served as a reference (black boxes). Please note that the P dopant concentration was lower compared to the structures shown in Fig. 3, thus, at  $T_{RTP} \geq 900$  °C, B was not overcompensated but  $\rho_c$  was high for the reference without DBI due to strong interdiffusion. All structures received the FA prior to a-Si:H(p $^+$ ) deposition and a final RTP step to ensure low-ohmic contact to the c-Si bulk and high sensitivity to differences directly at the SiTJ. Since  $\rho_c$  was low ( $<100$  m $\Omega$ cm $^2$ ) up to  $T_{RTP} = 850$  °C even without interlayer, most interlayers were only tested at  $T_{RTP} = 900$  °C and  $T_{RTP} = 950$  °C.

A 6-nm-thick B-doped SiC $_x$  interlayer (C content of  $\sim 40$  at%) seemed to hamper parasitic interdiffusion very efficiently, as very low  $\rho_c$  up to  $T_{RTP} = 900$  °C were measured (red boxes). At  $T_{RTP} = 800$  °C, the SiC $_x$  did not increase  $\rho_c$  compared to

the reference and a clear benefit is visible at 850 and 900 °C. At 950 °C, however,  $\rho_c$  degraded significantly and was of the same order of magnitude as the reference. With ultrathin (nominally 0.8 nm) ALD SiN $_x$  also very low  $\rho_c$  was obtained (blue boxes). In contrast to the SiC $_x$  interlayer,  $\rho_c$  was low even at  $T_{RTP} = 950$  °C, outperforming the reference structures by three orders of magnitude (24 m $\Omega$ cm $^2$  vs.  $\approx 2.0 \times 10^4$  m $\Omega$ cm $^2$ ). SiN $_x$  is known for its high density and is, thus, not easily penetrable and effectively blocks diffusion of various elements already at very low thicknesses [35]. Using a slightly thicker SiN $_x$  layer (nominally 1.5 nm) led to high  $\rho_c$  around  $10^3$  m $\Omega$ cm $^2$  independent of  $T_{RTP}$  (not shown). Since the diffusion blocking behavior should be as good or even better compared to the thinner SiN $_x$  layer, apparently the tunneling probability through the insulating SiN $_x$  was significantly decreased with increased SiN $_x$  thickness.

For SiO $_x$  interlayers similarly lower thickness was beneficial regarding  $\rho_c$  [“SiO $_x$ 1” vs. “SiO $_x$ 2” and “TO1” vs. “TO2,” Fig. 4(b)]. Besides thickness, the stoichiometry of the used oxide is decisive [21], [36]. Thermally grown TO2 was not only slightly thicker than TO1 (1.3 vs. 1.2 nm) but also comprised a higher oxygen content [21]. This makes TO2 less susceptible to the formation of pinholes as compared to TO1 [36], [37]. On one hand, pinholes can facilitate transport across the oxide. On the other hand, pinholes represent local dopant diffusion paths. Thus, the role of pinholes cannot definitively be answered here. While  $\rho_c$  for structures including TO1 was similar for both  $T_{RTP} = 900$  °C and 950 °C,  $\rho_c$  for TO2 was significantly higher compared to TO1 at  $T_{RTP} = 900$  °C but decreased to a similar level at  $T_{RTP} = 950$  °C.

Despite the more permeable matrix of wet-chemically grown HNO $_3$  oxide [21], similar results to TO1 samples were obtained when including it between n- and p-type poly-Si. A 0.8-nm-thick ALD SiO $_x$  (“SiO $_x$ 1”) interlayer provided similar  $\rho_c$  as the previously mentioned oxides in the range of 200–400 m $\Omega$ cm $^2$

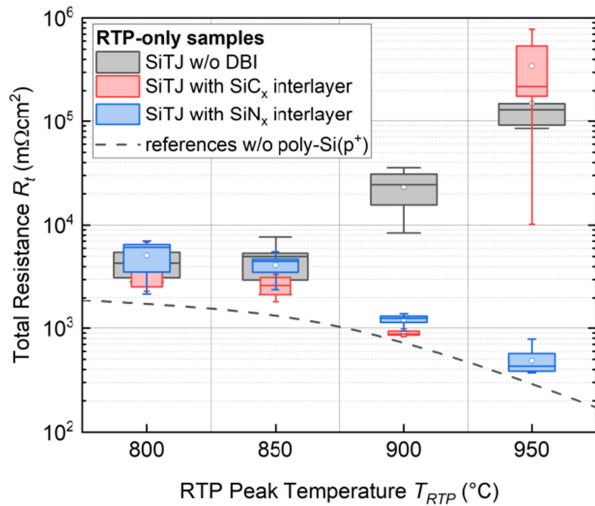


Fig. 5. Total resistance  $R_t$  of RTP-only SiTJs, including bulk and rear side contributions. As a guide to the eye, the trend of reference structures where the p-type Si deposition was omitted is represented by the dashed line.

at  $T_{RTP} = 900$  °C. However, at 950 °C the oxide seemed to be penetrated by dopants, as higher resistances were measured and no active n-type doping in the poly-Si(n<sup>+</sup>) was detected via ECV (not shown). Hence, in contrast to SiN<sub>x</sub>, 0.8 nm of ALD SiO<sub>x</sub> were apparently too thin to hold back dopants at this temperature. Moreover, the structure of ALD oxides might be less stoichiometric than that of thermal oxides, since a lower temperature has been used during the ALD process compared to thermal oxidation. This could be another reason why they are less effective diffusion barriers [21]. In [11], we reported that the initial deterioration of the passivation quality due to the RTP can be cured with a standard hydrogenation step. It is worth mentioning, while the passivation quality was not tested for the structures presented in Fig. 4, on similar sister samples the SiN<sub>x</sub> and SiC<sub>x</sub> interlayers (and presumably also the oxide interlayers) were found not to deteriorate the passivation quality of TOPCon and allowed for  $iV_{oc} \approx 725$  mV. It seems reasonable to assume that although the DBI blocks P and B diffusion, smaller hydrogen can still diffuse through it and passivate dangling bonds at the c-Si surface efficiently.

In the lean RTP-only process route (see Fig. 1), high  $T_{RTP}$  are necessary for the formation of a low-ohmic contact to the wafer [11]. By counteracting interdiffusion at these high temperatures with a suitable DBI, the realization of a low-resistive SiTJ stack on TOPCon with only one high temperature step might be possible. The most promising interlayers providing the lowest  $\rho_c$ , namely PECVD SiC<sub>x</sub> and 0.8 nm thick ALD SiN<sub>x</sub>, were, thus, also tested in the RTP-only route (Fig. 5). Note that Fig. 5 depicts the total resistance  $R_t$  of the structures including bulk and rear side contributions. Whereas the resistance of SiTJs without DBI increased drastically for  $T_{RTP} \geq 900$  °C, SiTJs with DBI followed the trend of decreasing  $R_t$  of reference structures where the poly-Si(p<sup>+</sup>) was omitted (dashed line in Fig. 5). The SiC<sub>x</sub> SiTJ was again degraded at  $T_{RTP} = 950$  °C, but the SiN<sub>x</sub> SiTJ was still stable at this temperature and provided a reasonable  $R_t$  of  $\approx 450$  mΩcm<sup>2</sup>. This value is mainly limited by the contact to

the wafer and not by the SiTJ. To allow better contact formation to the wafer with RTP-only, the thermally grown Si tunnel oxide was replaced with a wet-chemically grown SiO<sub>x</sub>. With this, a SiTJ with very low  $\rho_c = 30$  mΩcm<sup>2</sup> and high  $iV_{oc} = 711$  mV was achieved with a single fast high temperature step at  $T_{RTP} = 850$  °C (not shown). Unfortunately, in contrast to thermally grown oxides, the thermal stability of the wet-chemical oxide is limited to temperatures below 900 °C. Above 900 °C it cannot provide satisfying surface passivation anymore ( $iV_{oc} < 700$  mV) [21], [37]. Thus, the gain in  $\rho_c$  due to DBIs, which is highest at  $T_{RTP} \geq 900$  °C, cannot be exploited.

#### D. In-Depth Analysis of SiC<sub>x</sub> and SiN<sub>x</sub> Interlayers

To visualize diffusion and to distinguish between B and P, ToF-SIMS measurements were conducted on structures exposed to an RTP with  $T_{RTP} = 900$  °C. Please note that these samples were not exposed to the FA after a-Si:H(n<sup>+</sup>) and prior to a-Si:H(p<sup>+</sup>) deposition. The profiles were aligned by setting the maximum of the peak at the poly-Si/SiO<sub>x</sub>/c-Si interface to a depth of zero. A constant sputter rate was assumed in all layers to convert the sputter time into a sample depth. Without interlayer, P diffused heavily into the nominally p-type region, resulting in a high P concentration throughout both poly-Si layers [see Fig. 6(a)]. The profile evidently resembles the profiles after RTP at  $T_{RTP} = 900/950$  °C in Fig. 1(a). In contrast, the profile for the structure comprising the SiN<sub>x</sub> interlayer shows the high P diffusion blocking ability of SiN<sub>x</sub>. Consequently, the P plateau concentration in poly-Si(n<sup>+</sup>) was higher compared to the sample without interlayer. The SiC<sub>x</sub> interlayer also blocked P diffusion, as the P concentration dropped to background noise level in the p-type region. Nevertheless, the P concentration was lower throughout the entire poly-Si(n<sup>+</sup>) region. Presumably P atoms diffused into the 6-nm-thick SiC<sub>x</sub> layer but were slowed down and stopped there. Indeed, P enrichment in the SiC<sub>x</sub> layer was confirmed by a TEM EDX mapping (not shown).

B diffusion was also efficiently blocked by SiN<sub>x</sub> as the B concentration decreased steeply down to noise level within the first few nanometers of the poly-Si(n<sup>+</sup>) [see Fig. 6(b)]. On the contrary, with a SiC<sub>x</sub> interlayer, the B concentration decreased not as abruptly and reached deeper into the poly-Si(n<sup>+</sup>), similar to the B profile for the structure without interlayer. One reason why B diffusion is not as efficiently blocked by the SiC<sub>x</sub> might be that it is itself heavily B-doped. B diffusion was more pronounced at  $T_{RTP} = 950$  °C and resulted in an overcompensation of P in poly-Si(n<sup>+</sup>), as measured with ECV (not shown). Thus, the now completely p-type poly-Si formed a regular p/n junction with the n-type c-Si, explaining the very high  $\rho_c$  and diode-like  $J$ - $V$  characteristic of structures with SiC<sub>x</sub> interlayer at  $T_{RTP} = 950$  °C in Figs. 4(a) and 5.

TEM images were recorded to gain insight into the microstructure of the Si layers and the DBI forming the SiTJ. Fig. 7(a) shows a cross-section overview of both poly-Si layers of the SiTJ without DBI on top of the c-Si bulk. The bright contrast at the top left corner corresponds to a C protection layer deposited during lamella preparation. Noticeably, the interface between the p<sup>+</sup> and n<sup>+</sup> poly-Si layer is not visible. This could be



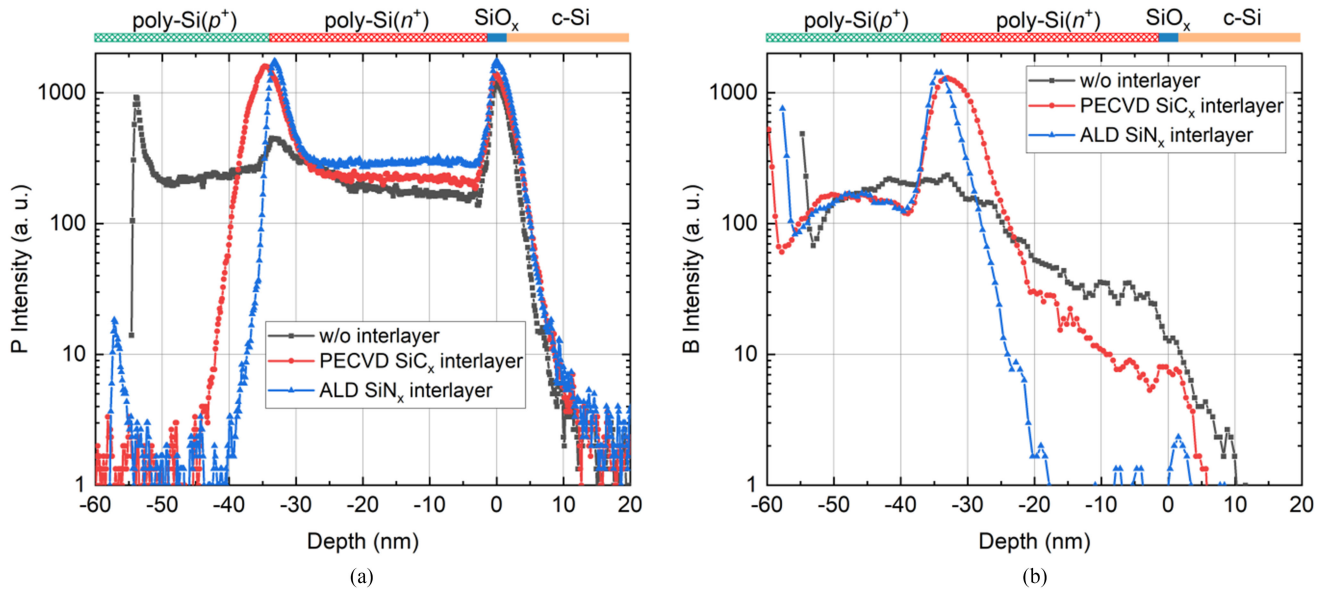


Fig. 6. (a) P and (b) B concentration as measured with ToF-SIMS of SiTJ comprising a PECVD SiC<sub>x</sub> interlayer or an ALD SiN<sub>x</sub> interlayer in comparison to an SiTJ without interlayer. All samples were exposed to an RTP with T<sub>RTP</sub> = 900 °C.

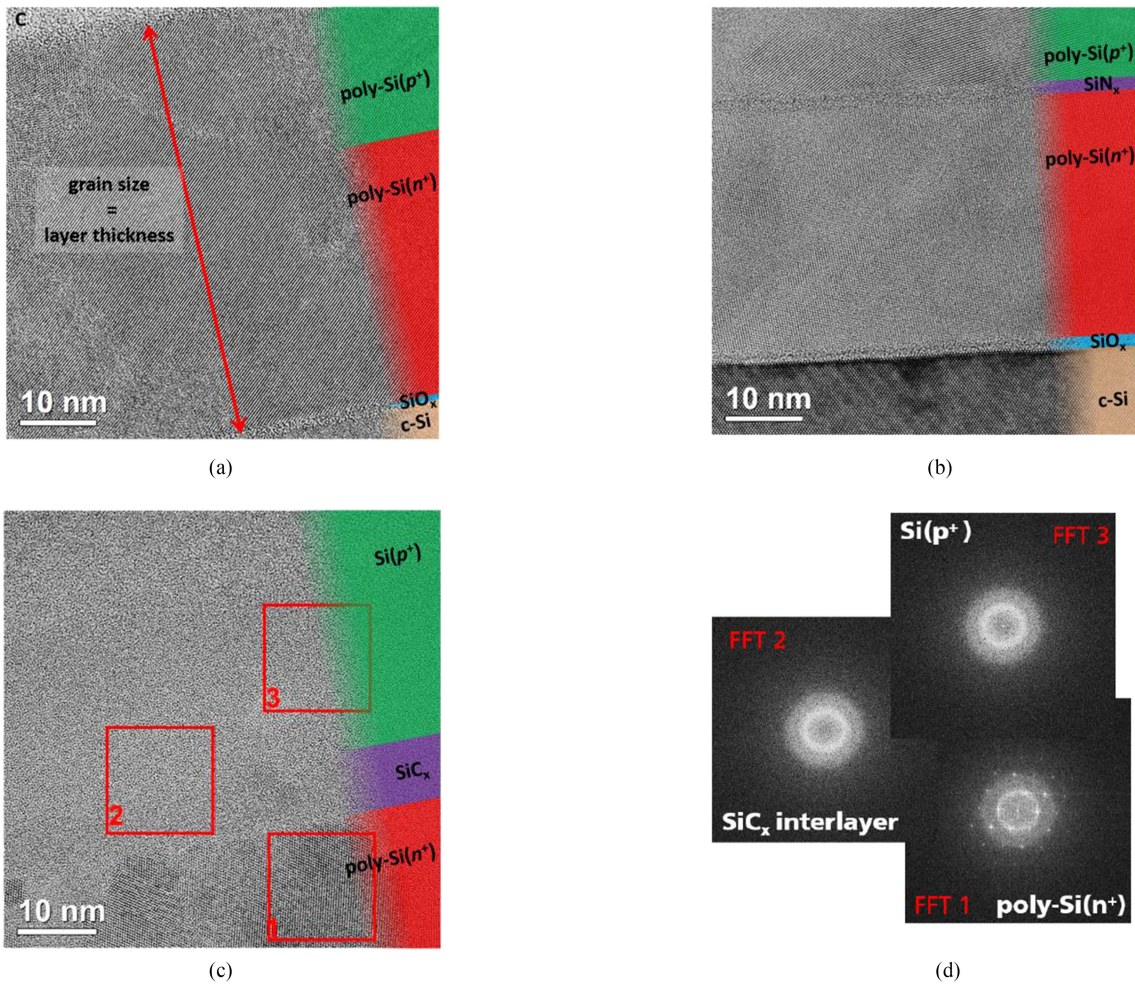


Fig. 7. Microstructure of the SiTJ (a) without DBI, (b) with SiN<sub>x</sub>, and (c), (d) with SiC<sub>x</sub> interlayer. (d) The FFT of the three red regions of interest in (c), representing the three different thin films. Colored areas in (a), (b), and (c) sketch the sample structure.

explained by a rather rough interface. In that case, the interface position would slightly vary across the thickness of the lamella ( $\sim 50\text{--}100$  nm) and clear projection of the interface would not be possible. Consequently, the native oxide at the SiTJ interface, visible in the ToF-SIMS profiles (Figs. 2 and 6), was not detected here. However, an EDX map of this area showed oxygen enrichment at the  $p^+/n^+$  interface (not shown). The amorphous, intentionally thermally grown  $\text{SiO}_x$  at the poly-Si/c-Si interface was clearly distinguished from the adjacent (poly-)crystalline Si [see Fig. 7(a)]. In some cases, crystal grains spread across the entire combined poly-Si layer thickness of roughly 50 nm. This shows that the SiTJ interface was not very distinct and the native oxide was not thick enough to separate both poly-Si layers. In general, dopant diffusion in poly-Si is much faster along grain boundaries compared to the migration through Si crystal grains [38], [39], thus large grains rather hamper diffusion. Nevertheless, grain boundaries spreading across the  $p^+/n^+$  Si interface might act as fast diffusion paths and facilitate parasitic interdiffusion.

On the cross-section overview of the SiTJ with  $\text{SiN}_x$  interlayer [see Fig. 7(b)], it is noticeable that the nitride layer is clearly visible, separating the different doped Si layers. Both the doped layers were clearly poly-crystalline, as without DBI. Again, in some cases, grains spread across the entire thickness of the respective poly-Si layer but were separated by the thin amorphous  $\text{SiN}_x$  interlayer.

Fig. 7(c) shows a cross-section of the SiTJ with  $\text{SiC}_x$  interlayer. On closer examination of the multilayer stack, significant differences appeared between the different layers. Whereas the P-doped layer was again clearly poly-crystalline, in the  $\text{SiC}_x$  and the B-doped Si layer no larger scale grains were visible [see Fig. 7(c)]. In the three red marked regions of interest, representing poly-Si( $n^+$ ) (FFT1), the  $\text{SiC}_x$  interlayer (FFT2), and Si( $p^+$ ) (FFT3), the signal was undertaken a fast Fourier transformation (FFT) to display the crystal lattice in reciprocal space [see Fig. 7(d)]. Note that FFT2 covers both  $\text{SiC}_x$  and Si( $p^+$ ). FFT1 showed circular brightness contrasts, corresponding to the amorphous phase with no long-range order, overlaid with a clear dot pattern, representing the lattice of the grain. FFT2 and FFT3 showed no sign of long-range order; only the amorphous phase was visible. For the  $\text{SiC}_x$  layer, this can be readily understood, since due to the high C content of roughly 40 at% crystallization was impeded and higher temperatures above  $900^\circ\text{C}$  are necessary to crystallize  $\text{SiC}_x$  with such a high C content [40]. The Si( $p^+$ ) layer was deposited subsequently without vacuum break, which lead to some C contamination (C content  $\sim 5\text{at}\%$ ) according to an EDX line scan (not shown). Nevertheless, very high active dopant concentrations  $N$  close to  $1.0 \times 10^{20} \text{ cm}^{-3}$  were measured with ECV in the Si( $p^+$ ) layer (not shown), which would not be possible in a completely amorphous layer [41], [42]. Since a TEM lamella represents only a small fraction of the whole sample, it might be possible that an amorphous section was selected coincidentally. This scenario is, however, very unlikely. Another important aspect is the orientation of the lamella to the incident electron beam. A crystal grain is only visible if the Bragg's law is fulfilled. Yet, although the lamella was tilted in several orientations, the image

was basically unchanged, and no crystal grains appeared. It is also possible that very small grains on the nanometer scale are present with a broad distribution of orientation, which would make them appear as amorphous phase or not detectable in the FFT. This could explain the high activation of dopants measured in ECV. Lastly, damage of the Si( $p^+$ ) layer during lamella preparation that caused its amorphization cannot be ruled out completely. Evidence for that is the further increased C content in the Si( $p^+$ ) layer close to the C protection layer detected via EDX and the rougher Si( $p^+$ ) surface compared to the lamella without DBI (not shown).

#### IV. CONCLUSION

A  $p^+/n^+$  poly-SiTJ based on TOPCon was presented. Depending on the applied thermal budget, significant interdiffusion of dopants was observed, limiting the SiTJ performance by drastically increasing  $\rho_c$  or by yielding an isotype structure due to complete overcompensation of one dopant species. Two approaches have been presented that prevent such parasitic interdiffusion and thereby improving the thermal stability of the SiTJ: C-alloying of the poly-Si layers and/or utilizing a DBI at the SiTJ. The ability to block P and B diffusion was studied for the most promising interlayers, ALD  $\text{SiN}_x$  and PECVD  $\text{SiC}_x$ . Further, the microstructure of the SiTJ was studied via TEM. It was also possible to show that a lean process sequence using only one single fast thermal treatment can enable a low-resistive and well-passivating SiTJ.

The improved thermal stability of the SiTJ eases its device integration such as into an industrially feasible Si bottom solar cell for tandem application based on PERC with the P-doped emitter replaced by a TOPCon front contact.

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