Passivation Enhancement of Poly-Si Carrier-Selective Contacts by Applying ALD Al$_2$O$_3$ Capping Layers

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Passivation Enhancement of Poly-Si Carrier-Selective Contacts by Applying ALD Al₂O₃ Capping Layers

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Abstract—Hydrogenation of polycrystalline silicon (poly-Si) passivating contacts is crucial for maximizing their passivation performance. This work presents the application of Al₂O₃ prepared by atomic layer deposition as a hydrogenation capping layer. Several important questions related to this application of Al₂O₃ are addressed by comparing results from Al₂O₃ single layers, SiNₓ single layers, and Al₂O₃/SiNₓ double layers to different poly-Si types. We investigate the effect of the Al₂O₃ thickness, the poly-Si thickness, the poly-Si doping type, and the postdeposition annealing treatment on the passivation quality of poly-Si passivating contacts. Especially, the Al₂O₃/SiNₓ stack greatly enhances the passivation quality of both n⁺ and p⁺ doped as well as intrinsic poly-Si layers. The Al₂O₃ layer thickness is crucial for the single-layer approach, whereas the Al₂O₃/SiNₓ stack is less sensitive to the thickness of the Al₂O₃ layer. A thicker Al₂O₃ layer is needed for effectively hydrogenating p⁺ compared to n⁺ poly-Si passivating contact. The capping layers can hydrogenate poly-Si layers with thicknesses up to at least 600 nm. The hydrogenation-enhanced passivation for n⁺ poly-Si is found to be more thermally stable in comparison to p⁺ poly-Si. These results provide guidelines on the use of Al₂O₃ capping layers for poly-Si contacts to significantly improve their passivation performance.

Index Terms—Atomic layer deposition (ALD) Al₂O₃, hydrogenation, passivation quality, polycrystalline silicon (poly-Si) passivating contacts, thermal stability.

I. INTRODUCTION

CRYSTALLINE silicon (c-Si) solar cells with polycrystalline silicon (polysilicon) as passivating contacts enable record-high efficiencies due to their excellent passivation and carrier selectivity [1]–[8]. This type of contact consists of an ultrathin SiOₓ layer and a heavily doped polycrystalline Si layer on top. So far, most work has focused on improving the quality of poly-Si passivating contacts [9]–[14] and enhancing cell efficiencies. Furthermore, the carrier transport mechanism has been studied as well [15]–[18]. Hydrogenation plays a crucial role in the poly-Si contact formation to achieve outstanding passivation quality [19]–[25]. However, publications that focus specifically on the hydrogenation of poly-Si passivating contacts [8], [10], [19], [25], [28] are fairly limited in comparison to the publications that focus on the development of poly-Si passivating contacts and their application in solar cells [7], [11], [16], [24], [29]–[33]. The passivation of c-Si surfaces by poly-Si relies on two mechanisms: 1) field-effect passivation and 2) chemical passivation [34]. The field-effect passivation is due to the difference in doping level between the heavily doped poly-Si and the lightly doped c-Si bulk, which induces band bending at their interface. This band bending reduces the minority carrier concentration, which, in turn, reduces surface recombination. To maximize this interface band bending, one needs to optimize the doping profile near the poly-Si/SiOₓ/c-Si interfaces. On the other hand, an optimum doping profile is necessary but not sufficient in attaining the highest passivation quality. This is because of the thin SiOₓ layer (typically ≤ 2.2 nm) located between c-Si and poly-Si that is also a crucial factor in the passivation quality. The SiOₓ material properties, such as its microstructure as well as its atomic and chemical composition, depend on the preparation method. However, irrespective of the type of SiOₓ layer that is used, there always remain some Si bonds at the interface that are not terminated, i.e., Si dangling bonds, and these can act as recombination centers that degrade the chemical passivation [10]. Therefore, an extra step is necessary to passivate these dangling bonds and an effective way to achieve this is by the introduction of hydrogen [7], [35]–[38]. Hydrogenation can be realized with H₂ gas during annealing [34], by a hydrogen-containing remote plasma [39] or by hydrogen-containing capping layers, for example, PECVD SiNx [4], [28] and atomic layer deposition (ALD) Al₂O₃ and TCO layers followed by thermal annealing [10], [34], [37], [40]–[44]. SiNx and Al₂O₃ are common materials that are used for surface passivation of c-Si [30], [45], [46]. When annealed at a sufficiently high temperature, the hydrogen in the capping materials can diffuse through the poly-Si materials and passivate the Si-dangling bonds at the SiOₓ/c-Si interface. Although they
have proven to be effective capping layers for hydrogenation, more practical insights into the application of the Al<sub>2</sub>O<sub>3</sub>-based capping layers on hydrogenating of poly-Si carrier selective contacts should be obtained, which is the focus of this work.

To decouple the influence of the field-effect passivation due to the heavy doping of the poly-Si layers from the influence of the chemical passivation owing to the hydrogen passivation, different types of poly-Si (intrinsic, n<sup>+</sup>, and p<sup>+</sup> type) were studied in this work. Furthermore, the dependence of the poly-Si passivation enhancement induced by several parameters used during the hydrogenation process has not been clarified thus far. Therefore, we have studied different capping layers (including ALD Al<sub>2</sub>O<sub>3</sub>, PECVD SiN<sub>x</sub>, and Al<sub>2</sub>O<sub>3</sub>/SiN<sub>x</sub> double-layer capping) with a focus on the influence of the Al<sub>2</sub>O<sub>3</sub> thickness, the PECVD SiN<sub>x</sub> layer, the poly-Si layer doping types and thicknesses, and the annealing temperature. Finally, the thermal stability of the enhanced poly-Si passivation enabled by different types of hydrogenation approaches was analyzed.

II. EXPERIMENT

Double-side polished n-FZ wafers with a resistivity of 1-5 Ω·cm and <100> orientation were used in this work. The thickness of the wafers before texturing with TMAH (trimethylaluminium hydroxide) was 280 ± 20 μm. On all symmetrical passivation test samples, a thin SiO<sub>x</sub> layer was grown by nitric acid oxidation of silicon (NAOS) [45] or thermal oxidation (th-SiO<sub>x</sub>) [31]. Subsequently, intrinsic LPCVD poly-Si (i/poly-Si) layers were deposited on both sides. The deposition time was adjusted for poly-Si deposition on textured c-Si surfaces to obtain a poly-Si layer with an effective thickness of 150 nm, which is the same as that on flat c-Si surfaces. Doping was introduced via phosphorous ion implantation on both sides of the samples with the energy of 20 keV and dose of 6 × 10<sup>15</sup> cm<sup>-2</sup> for n<sup>+</sup> poly-Si [45] or via BBr<sub>3</sub> diffusion for p<sup>+</sup> poly-Si [31]. For the n<sup>+</sup> poly-Si, a subsequent high-temperature annealing treatment at 950 °C for 5 min was applied to activate and diffuse the dopants.

To study the dependence of the hydrogenation on the poly-Si layer thickness, poly-Si samples with different thicknesses were prepared. For these n<sup>+</sup> poly-Si samples with different thicknesses, the same high-temperature annealing process was used to activate the ion-implanted phosphorus. Due to the differences in the poly-Si layer thickness, different phosphorous doping profiles at the c-Si/SiO<sub>x</sub>/poly-Si interfaces can be expected for these samples as was shown in our previous study [32], which should, in turn, induce differences in the levels of field-effect passivation. All the samples used in this work were one-quarter of 4-in. round wafers, which were cut before the deposition of the capping layer(s).

Three hydrogenation approaches were compared in this work: 1) ALD Al<sub>2</sub>O<sub>3</sub> capping layers with different thicknesses; 2) PECVD SiN<sub>x</sub> capping layers; 3) Al<sub>2</sub>O<sub>3</sub>/SiN<sub>x</sub> double-capping layers.

An HF dip was conducted before the deposition of the capping layers. The Al<sub>2</sub>O<sub>3</sub> layers were deposited by thermal ALD in an Oxford Instruments OpAL reactor at a substrate temperature of 200 °C. Trimethylaluminum [Al(CH<sub>3</sub>)<sub>3</sub>] and H<sub>2</sub>O were used as the metal precursor and coreactant, respectively. The ALD cycle time was ~7 s and the growth per cycle was 1.1 Å [46]. The ALD cycles were repeated until the target film thicknesses (from 2 to 16 nm) were reached. The SiN<sub>x</sub> layers were deposited in an Oxford Instruments PECVD reactor at a substrate temperature of 400 °C with SiH<sub>4</sub> and NH<sub>3</sub> as precursors. The deposition rate was 15 nm/min for flat surfaces. To obtain similar SiN<sub>x</sub> layer thicknesses for flat and pyramid textured Si surfaces, the deposition time for textured samples was multiplied by 1.73 to account for the difference in an effective area between the pyramid textured facets and flat surfaces.

After deposition of the capping layers, all samples received an annealing treatment at 400 °C for 30 min in forming gas (10% H<sub>2</sub> in N<sub>2</sub> atmosphere, also known as forming gas annealing, FGA) before measuring the passivation quality. Different FGA temperatures and times were used to test the thermal stability of the passivation quality achieved by the aforementioned hydrogenation approaches. The lifetime and implied open-circuit voltage (iV<sub>OC</sub>) of the samples were analyzed in a Sinton WCT-120 lifetime tester applying the generalized measurement mode [47].

III. RESULTS

We first studied the influence of the poly-Si doping type on the enhancement of the passivation quality for poly-Si samples with different hydrogenating capping layers. For i/poly-Si, the initial passivation levels are very low, with an iV<sub>OC</sub> of 545 mV before any hydrogenation process, see Fig. 1. By capping the sample with 2-nm-thick Al<sub>2</sub>O<sub>3</sub> and conducting a subsequent FGA, the passivation quality is slightly enhanced. The enhancement of the passivation quality that is induced by a 75-nm-thick SiN<sub>x</sub> layer followed by an FGA treatment is much larger, resulting in a clear increase in minority carrier lifetime and an iV<sub>OC</sub> of 650 mV. However, when combining both materials in the form of a 2-nm-thick Al<sub>2</sub>O<sub>3</sub> layer covered with a 75-nm-thick SiN<sub>x</sub> capping layer, we observe the largest enhancement of the passivation quality for i/poly-Si. The minority carrier lifetime of this sample almost reaches 1 ms with an iV<sub>OC</sub> of 694 mV. When
et al. and Al doped and (b) p doped poly-Si on planar capping layer approaches, as a function of the p doping and Al double cap-layer the passivation quality poly-Si followed by FGA treatment doped poly-Si surface and layer thickness, we choose samples cm as interlayer, the three different hybrid layer thickness generally enhances the passivation values and, therefore, is not providing poly-Si samples with poly-Si prepared on a textured c-Si surface with th-SiO$_3$ as interfacial SiO$_3$. For the curves.

![Fig. 2. Effective lifetime as a function of minority carrier density (MCD, the injection level) of the symmetrical test samples before hydrogenation and after hydrogenation for 150-nm thick (a) n$^+$ doped and (b) p$^+$ doped poly-Si prepared on flat c-Si surfaces with NAOS as interfacial SiO$_3$, and (c) 150-nm p$^+$ doped poly-Si prepared on a textured c-Si surface with th-SiO$_3$ as interfacial SiO$_3$. For all the samples with the capping layer(s), an FGA step at 400 °C is carried out before the lifetime measurement. The doping levels for B and P are higher than 1 × 10$^{20}$ cm$^{-3}$; the doping profiles of the n$^+$ and p$^+$ doped poly-Si samples are given in [33] and [64]. The MCD at MPP [48] and the point and value of the one-sun implied open-circuit voltage (i$V_{OC}$) are calculated and indicated for the curves.

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comparing the same hydrogenation approaches for n$^+$ and p$^+$ doped poly-Si samples, we also find that the Al$_2$O$_3$/SiN$_x$ double capping layer performs the best, as shown in Fig. 2(a) and (b). Due to the presence of field-effect passivation introduced by the heavy doping within the poly-Si, as well as a possible gettering effect by the dopants, the lifetime measured for both doped samples before hydrogenation is much higher in comparison to the (i)poly-Si sample. For n$^+$ and p$^+$ doped poly-Si on planar surfaces, we find that the enhancement in passivation quality by applying a 75-nm-thick SiN$_x$ followed by FGA treatment is small compared to the approaches of a single Al$_2$O$_3$ (8 nm) capping layer or an Al$_2$O$_3$ (8 nm)/SiN$_x$ (75 nm) double capping layer. In order to see whether the abovementioned trends, obtained on a flat c-Si surface with NAOS-SiO$_3$ as interlayer, are invariant of the type of c-Si surface morphology and the preparation method of SiO$_3$ interlayer, the three different hydrogenation approaches were also tested for a more challenging case, i.e., p$^+$ poly-Si on textured Si surfaces with thermal-SiO$_2$ as interlayer, see Fig. 2(c). We find that a 75-nm-thick SiN$_x$ layer with a subsequent FGA can hydrogenate the p$^+$ poly-Si samples well, but also in this case, with an extra 8-nm-thick Al$_2$O$_3$ layer between the p$^+$ poly-Si and the SiN$_x$ layer the passivation quality is enhanced the most when looking at the high injection level around maximum power point (MPP) [48].

In order to study the dependence of the passivation quality enhancement on the Al$_2$O$_3$ layer thickness, we choose samples with three cases: n$^+$ and p$^+$ doped poly-Si on a flat surface that gives the high passivation quality and p$^+$ doped poly-Si on a textured surface, which gives the lowest passivation quality. The results are shown in Fig. 3. We found that an FGA treatment does not yield very high i$V_{OC}$ values and, therefore, is not providing adequate passivation. The capping by Al$_2$O$_3$ or Al$_2$O$_3$/SiN$_x$ followed by annealing enhances the passivation performance significantly. In both these hydrogenation approaches, increasing the Al$_2$O$_3$ layer thickness generally enhances the passivation quality up to a thickness of around 8 nm. A further increase in the Al$_2$O$_3$ layer thickness does not help in enhancing the passivation quality, except for textured p$^+$ poly-Si samples with an Al$_2$O$_3$ single capping layer. Considering that the Al$_2$O$_3$ thicknesses are the same on the flat p$^+$ poly-Si surface and the textured p$^+$ poly-Si facets due to the excellent conformality of the ALD technique, we conclude that textured p$^+$ poly-Si...
samples need a thicker Al$_2$O$_3$ layer for a further enhancement of the passivation quality. Furthermore, the fact that the dependence of the enhancement in passivation quality on the Al$_2$O$_3$ layer thickness is more pronounced for $p^+$ on the textured surface than it is for $p^+$ and $n^+$ poly-Si samples on flat surfaces can also be related to the difference between planar and textured surfaces. Comparing the two hydrogenation approaches shown in Fig. 3, for both $n^+$ and $p^+$ poly-Si samples, the Al$_2$O$_3$/Si$_N_x$ approach presents a larger enhancement in comparison to the single Al$_2$O$_3$ capping layer approach.

In order to study the dependence of the hydrogenation-induced passivation enhancement on the poly-Si layer thickness, we intentionally prepared samples with a large variation in the poly-Si layer thicknesses. First, we selected a type of $n^+$ poly-Si, which was optimized for a 300-nm-thick poly-Si sample in terms of doping profile for achieving the highest field-effect passivation before hydrogenation. Next, we used the same process parameters, i.e., the same NAOS-SiO$_x$, P-implantation, and high-temperature annealing to prepare samples with different poly-Si thicknesses (50, 150, and 600 nm). As a consequence, these samples are not prepared at their optimum conditions, in terms of implantation and annealing parameters. Especially for the thin poly-Si samples, when using the same implantation and annealing parameters as that for the optimized 300-nm-thick poly-Si sample, a much deeper and higher doping level of P in-diffusion to the c-Si bulk is expected, which was already observed in our previous work [32]. Therefore, lower passivation qualities are obtained for these samples than that for the optimized 300-nm-thick poly-Si one, see Fig. 4. Since the Si$_N$$_x$ layer is commonly used in TOPCon solar cells, for example, the i-TOPCon [65], as hydrogenation and antireflection layer, we presented the passivation results of poly-Si samples prepared with 75-nm-thick Si$_N$$_x$ and Al$_2$O$_3$(8 nm)/Si$_N$$_x$(75 nm) hydrogenation approaches, which can be seen in Fig. 4. Again, the Al$_2$O$_3$/Si$_N$$_x$ double capping layer approach gives a larger enhancement in passivation than the Si$_N$$_x$ single capping layer approach. Moreover, for the optimized 300-nm-thick flat $n^+$ poly-Si, the enhancement due to the hydrogenation is less clear, when compared to the nonoptimized samples. Especially for the 150-nm-thick poly-Si sample, the enhancement is very pronounced, which brings its passivation quality back to the trend of their dependence on the poly-Si thickness.

In the previous work, the hydrogenation-induced passivation quality proved to be thermally stable against a metal paste firing process [30]. However, the exposure of the poly-Si samples at the firing peak temperature is only a few seconds. To find the threshold thermal budget that degrades the hydrogenation effect and to compare the hydrogenation approaches in this respect, we also tested the thermal stability of the passivation quality after hydrogenation with Al$_2$O$_3$ or Al$_2$O$_3$/Si$_N$$_x$ capping approaches.

The accumulative annealing treatments used for these tests were conducted in forming gas with different thermal budgets. As shown in Fig. 5(a), the passivation quality in the case of flat $n^+$ poly-Si can withstand a 30-min-long FGA treatment at 600 °C. However, when increasing the annealing temperature to 700 °C, even after only 5 min of FGA, the $n^+$ poly-Si loses its passivation quality. This is especially the case for the single Al$_2$O$_3$ capping layer approach, whereas the sample with a double capping approach.
layer still shows good passivation quality with $iV_{OC}$ exceeding 710 mV. In this respect, the $\text{Al}_2\text{O}_3/\text{SiN}_x$ double-layer capping appears to be more thermally stable than the single $\text{Al}_2\text{O}_3$ capping layer, in addition to also enabling a higher passivation quality. For $p^+$ poly-Si on a textured surface, see Fig. 5(b), the high passivation quality is maintained after a 30-min-long FGA treatment at 500 °C. However, when using a higher annealing temperature, e.g., 30-min-long FGA at 600 °C or 5-min-long FGA at 700 °C, a deterioration of the passivation quality is observed for both the single $\text{Al}_2\text{O}_3$ and $\text{Al}_2\text{O}_3/\text{SiN}_x$ double-layer capping approaches. The obtained $iV_{OC}$ values are below 680 mV, similar to the values reported before hydrogenation in Fig. 3.

IV. DISCUSSION

The field-effect passivation established on the c-Si surface using (i)poly-Si is very weak and the overall passivation is largely governed by chemical passivation provided by the tunnel SiO$_2$ layer. By passivating the Si-dangling bonds at the poly-Si/SiO$_2$/c-Si interface with hydrogen, an enhanced level of chemical passivation is found, as shown in Fig. 1. For the (i)poly-Si samples, we compared the hydrogenation effects of the abovementioned three different approaches. The minor enhancement of $iV_{OC}$ to 550 mV for the approach of $\text{Al}_2\text{O}_3$ capping followed by FGA is mainly due to the limited chemical passivation enhancement by the ultrathin $\text{Al}_2\text{O}_3$ capping layer which is only 2-nm thick [46], [49], [50]. When increasing the $\text{Al}_2\text{O}_3$ thickness to 32 nm, the $iV_{OC}$ increased to 687 mV (the expected to 550 mV for the approach of Al$^+$ poly-Si benefits more from a 75-nm-thick poly-Si layer thickness. At a certain FGA condition, a thicker Al$^+$ single capping layer to 8 nm while a single capping layer is needed to obtain optimized passivation. This means that when the $\text{Al}_2\text{O}_3$ thickness exceeds the aforementioned saturation threshold, the amount of hydrogen in the capping layer(s) is not the dominating factor for hydrogenating $n^+$ and $p^+$ poly-Si on flat surfaces. The way that hydrogen is bonded in the $\text{Al}_2\text{O}_3$ and released from the film seems also to play a very important role for the effective passivation induced by the $\text{Al}_2\text{O}_3$ as has also been discussed for passivation of c-Si before [50], [58]. For the case of textured Si surfaces, the passivation quality provided by $p^+$ poly-Si benefits more from a 75-nm-thick SiN$_x$ single capping layer than from an 8-nm-thick $\text{Al}_2\text{O}_3$ single capping layer, as shown in Fig. 2(c). This could possibly be related to the differences between $<111>$-oriented surfaces and $<100>$-oriented surfaces [59] as well as to a larger surface area for the textured surface (also due to the presence of nanotextures on the pyramid facets). For the textured surface, we speculate that the amount of hydrogen diffused from the 8-nm-thick $\text{Al}_2\text{O}_3$ layer into the c-Si surface with the applied annealing processes is not enough to reach the “saturation threshold.” In order to enhance the passivation, a higher amount of hydrogen is required to increase the probability of forming Si-H bonds to terminate the Si dangling bonds. The larger content of hydrogen within the 75-nm-thick SiN$_x$ layer compared to the 8-nm-thick $\text{Al}_2\text{O}_3$ layer could be helpful in this respect. This would be consistent with the results shown in Fig. 3, in the sense that the amount of hydrogen within the 16-nm-thick $\text{Al}_2\text{O}_3$ single capping layer that diffuses to the c-Si/SiO$_2$/poly-Si interface is still not enough to fully hydrogenate the sample with $p^+$ poly-Si on a textured Si surface. This implies that in the case of textured $p^+$ poly-Si samples more hydrogen is needed to hydrogenate the interfaces compared to what is needed for flat samples.

It is found that by applying an FGA treatment at 400 °C for 30 min, the $\text{Al}_2\text{O}_3$ single capping layer approach for hydrogenating flat poly-Si samples is better than the SiN$_x$ single capping layer. As a consequence, a higher passivation enhancement can be expected for the $\text{Al}_2\text{O}_3$/SiN$_x$ double capping layer approach, which combines the better hydrogenation capability from the...
Al₂O₃ capping layer with the higher hydrogen content properties from SiNₓ layers. This is an approach that is similar to what is used for c-Si surface passivation, by the Al₂O₃/SiNₓ double-layer [60]. It is found that for all cases considered here, irrespective of the poly-Si doping type or the c-Si surface morphology (see Figs. 1–3), the Al₂O₃/SiNₓ double capping layer hydrogenation approach yields the highest passivation quality. For flat n⁺ poly-Si samples, the SiNₓ capping makes it possible to reduce the Al₂O₃ layer thickness from 8 to 2 nm while still obtaining the highest passivation enhancement compared to the Al₂O₃ single capping layer approach. For samples with p⁺ poly-Si on textured Si surfaces with the SiNₓ capping, an 8-nm-thick Al₂O₃ layer is enough to achieve the highest passivation enhancement. This means that when applying a SiNₓ layer on top of Al₂O₃, the dependence of the hydrogenation effect on the Al₂O₃ thickness becomes less pronounced. However, the presence of Al₂O₃ is crucial for obtaining the best level of hydrogenation, as can be concluded from a comparison of the SiNₓ single capping approach to the Al₂O₃/SiNₓ double capping layer approach. It is especially true for the (i)poly-Si samples, even though the Al₂O₃ is as thin as 2 nm. As mentioned, it is not just related to the amount of hydrogen present in the stack, the way that hydrogen is bonded in the Al₂O₃ and released from the film during annealing seems to play a very important role too. The fact that a thin SiOₓ layer (< 2 nm) develops at the poly-Si/Al₂O₃ interface during the deposition and annealing processes and that there is a difference in fixed charges for the Al₂O₃/SiNₓ and SiNₓ cases is not expected to play a significant role. The surface recombination mainly happens at the c-Si/SiOₓ/(i)poly-Si interface and the depletion region induced by the fixed charges within the capping layer is expected not to extend to the c-Si surface for the 150-nm-thick (i)poly-Si.

As shown in Figs. 1 and 2, the passivation quality of poly-Si samples of all the doping types can be enhanced by the applied hydrogenation approaches. As discussed earlier, the Al₂O₃/SiNₓ stack is a highly effective hydrogenation approach for both intrinsic and doped (n⁺ and p⁺) poly-Si samples. Compared to the (i)poly-Si samples, the doped poly-Si samples show much higher passivation qualities due to the presence of the field-effect passivation and potentially due to the differences in the type and density of defects in the ultra-thin SiOₓ layer, which becomes doped with P (SiOₓ:P) or B (SiOₓ:B) after diffusion. The latter is, however, expected to be the same for samples with the same doping type, independent of the deposition of hydrogenating capping layer(s) leading to hydrogenation. On the other hand, due to the presence of the field-effect passivation in the doped poly-Si samples, the absolute gain in iV_{OC} values due to hydrogenation is not as high as it is for the (i)poly-Si samples.

An additional strong benefit of hydrogenation is that it can minimize variations in passivation levels due to nonoptimal doping processes or variations in a poly-Si layer thickness. Because the same process steps were used for all the samples shown in Fig. 4, when varying the poly-Si layer thickness, the doping profile (for thinner poly-Si samples) and doping level (for thicker poly-Si samples) will not be as optimal as that in the optimized 300-nm-thick poly-Si sample. If we assume that the ultra-thin SiOₓ:P interlayers are all similar for all the n⁺ poly-Si samples, the doping profile and level differences lead to the field-effect passivation quality differences between samples, therefore, their overall passivation qualities. Therefore, the field-effect passivation qualities of these nonoptimized samples are not as high as the optimized case, the 300-nm poly-Si sample, which can be seen from the differences in iV_{OC} values of these samples before hydrogenation, shown in Fig. 4. However, after hydrogenation, the enhancement in overall passivation quality of the optimized 300-nm-thick n⁺ poly-Si sample is less pronounced when compared to the nonoptimized samples, especially for the 150-nm-thick poly-Si sample. Interestingly, after hydrogenation, the ΔiV_{OC} values from wafer to wafer due to the poly-Si thickness variation, between 50 and 600 nm, are suppressed. This indicates that an effective hydrogenation process, which maximizes the chemical passivation, can partly compensate for a relatively poor field-effect passivation and induce a high overall passivation quality.

Due to the fact that a 75-nm-thick SiNₓ layer acts as a hydrogen effusion barrier for the Al₂O₃ layer, capping the Al₂O₃ layer with SiNₓ should be more thermally stable against the hydrogen loss during a high-temperature treatment. This is indeed observed for n⁺ poly-Si samples, as is shown in Fig. 5(a). A smaller drop in passivation quality is observed for the sample capped with an Al₂O₃/SiNₓ double capping layer when compared to the sample with a single Al₂O₃ capping layer after annealing at 700 °C for 5 min. However, for the 150-nm-thick p⁺ poly-Si on a textured Si surface, a similar trend is observed for both hydrogenation approaches [see Fig. 5(b)] and the drop in passivation quality is observed at a lower temperature in comparison to the n⁺ poly-Si sample. Despite the difference in poly-Si thickness, we believe this is not the dominant factor for de-hydrogenation/effusion of hydrogen for these poly-Si samples, since these poly-Si layer thickness values are higher than that for the capping layers. Also since our samples are capped, the H effusion is likely limited by the capping layer rather than the poly-Si layer thickness. Therefore, we conclude that n⁺ poly-Si is more thermally stable than p⁺ poly-Si. This may be due to the fact that hydrogen incorporation is less thermally stable in p⁺ poly-Si compared to n⁺ poly-Si. Something similarly has been reported for a-Si:H(p) and a-Si:H(n) in silicon heterojunction (SHJ) interfaces [61]. In the SHJ structure, hydrogen effusion is more energetically favorable for p-type a-Si:H, when E_F is close to the valence band, which induces lower thermal stability in comparison to n-type a-Si:H. For the hydrogenated p⁺ poly-Si samples, it still needs to be clarified whether the observed lower thermal stability for p⁺ poly-Si samples compared to n⁺ poly-Si samples can be attributed to similar reasons [26], [27], [42], [62], [63]. Obviously, the overall passivation quality provided by the Al₂O₃/SiNₓ double capping layer approach is not significantly better than the Al₂O₃ single-layer approach for p⁺ poly-Si. With a better understanding of the thermal stability of the hydrogenation-enhanced passivation, the superior performance of the double-layer approach may become apparent also in the case of p⁺ poly-Si.
V. CONCLUSION

In this work, the application of ALD AlOx as a hydrogenation capping layer for poly-Si is extensively studied. Hydrogenation approaches for poly-Si capped by ALD Al2O3, PECVD SiNx, and ALD AlOx combined with PECVD SiNx are compared. Application of any of these capping layers to n+, p+, and (i)poly-Si will result in an enhancement of the passivation quality. The final passivation quality strongly depends on the ALD Al2O3 thickness in the case of a single capping layer approach, whereas this is much less pronounced for the ALD Al2O3/SiNx stack, especially in the case of n+ poly-Si samples. The Al2O3/SiNx stack was demonstrated to be the most effective approach for hydrogenating poly-Si among all of the tested hydrogenation approaches. Nonoptimal field-effect passivation quality due to the doping or variations in poly-Si thickness can be compensated by effective hydrogenation, which induces a high level of chemical passivation. Additionally, capping the Al2O3 layer with SiNx, which acts as a hydrogen effusion barrier, improves the thermal stability of the hydrogenated n+ poly-Si samples. These findings show a promise for the application of the ALD Al2O3/SiNx stack for the effective hydrogenation of poly-Si-based passivating contacts.

REFERENCES


