

# Enhancing industrialization TOPCon solar cell efficiency via comprehensive anti-reflection passivation film optimization

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## ABSTRACT

This study focuses on enhancing the performance of n-type Tunnel Oxide Passivated Contact (TOPCon) solar cells by exploring the optimization of both front and rear film layers. For the front film, we implement a one-step plasma oxidation process before depositing silicon nitride on alumina, aiming to enhance the quality of the alumina layer and improve overall passivation. In the case of the rear film, we introduce a  $\text{NH}_3$  plasma treatment to elevate hydrogen content of  $\text{SiN}_x$ . These additional hydrogens diffuse into the interfacial silicon oxide during the firing process to help reduce the number of surface dangling bonds and inhibit the degradation of the passivating contacts, which significantly contributes to enhanced passivation quality. Through separate optimization of these film layers, we aim to harness the full potential of TOPCon solar cells, achieving remarkable improvements in passivation quality and overall performance. With the help of XRD, SIMS, QSSPC, ellipsometry and other characterization tools, the underlying reasons for the improved passivation quality due to plasma oxidation and plasma hydrogenation were explored. Finally, plasma oxidation and hydrogenation lead to  $\sim 0.06$  and  $\sim 0.07\%$  average efficiency enhancements, respectively.

## 1. Introduction

In recent years, significant advancements have been made in solar cell technologies, with the introduction of Tunnel Oxide Passivated Contact (TOPCon) solar cells being one of the most noteworthy breakthroughs [1–5]. TOPCon solar cells have exhibited superior efficiency and passivation properties compared to traditional silicon solar cells, making them an attractive option for large-scale photovoltaic applications. The core of the TOPCon comprises an ultra-thin oxide layer and a heavily doped polycrystalline silicon layer, which enables selective carrier transport, resulting in a combination of outstanding passivation quality and contact performance [6–8]. Regrettably, the application of this passivating contact on the solar cell front side presents challenges due to its intense light parasitic absorption, primarily attributed to the heavily doped polysilicon layer [9]. Indeed, in the current TOPCon solar cell continues the design of traditional solar cells, the front structure employs a boron homogeneous/selectivity emitter in combination with

passivation and anti-reflection film layers, such as alumina ( $\text{AlO}_x$ ) and silicon nitride ( $\text{SiN}_x$ ) [10,11]. Furthermore, the polysilicon passivating contact structure, when subjected to the firing process required for metallization, can suffer from substantial degradation in passivation quality [12]. To address this issue, a frequent practice is to shield the polysilicon with a hydrogen-rich  $\text{SiN}_x$  film, which effectively prevents the occurrence of passivation quality degradation and leads to a notable improvement in the overall passivation performance, due to the presence of hydrogen [13]. The significance of hydrogen content in the structural performance of doped polysilicon passivating contacts has been well-documented in extensive studies. It has been consistently shown that maintaining a higher concentration of hydrogen in the vicinity of the ultrathin oxide layer, achieved through various methods, can significantly enhance passivation quality [14–17]. And finally leading to a notable improvement in the electrical performance of TOPCon solar cells [18].

In this work, our primary objective was to optimize the front and rear

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stacked passivation films independently for TOPCon solar cells, with the aim of enhancing their overall passivation quality. The passivation film on the front side of the TOPCon solar cell consists of five distinct layers, arranged from bottom to top as follows:  $\text{AlO}_x$ , two layers of  $\text{SiN}_x$  with different refractive indices  $n$ , silicon nitride oxide ( $\text{SiO}_x\text{N}_y$ ), and a silicon oxide ( $\text{SiO}_x$ ). This specific combination of layers has been widely adopted by mainstream TOPCon solar cell manufacturers due to its dual benefits in optics and electricity. It effectively achieves excellent surface passivation, minimizing recombination losses, while also providing a notable anti-reflective effect. On this foundation, a one-step plasma oxidation process was implemented prior to depositing  $\text{SiN}_x$  on  $\text{AlO}_x$ . The purpose of this process was to eliminate oxygen vacancy defects within the  $\text{AlO}_x$  layer, thus improving its passivating properties. For the rear passivation, a combination of three layers of silicon nitride with different  $n$  is used to achieve both passivation and optical performance. As a further optimization, a  $\text{NH}_3$  plasma treatment was introduced to increase the hydrogen content before each layer of  $\text{SiN}_x$  deposition. Through this separate optimization of the front and rear film layers, better passivation quality can be observed without affecting the optical properties and the contact of the metal electrode with the silicon substrate. Finally, open-circuit voltage ( $V_{oc}$ ) enhancement due to improved passivation quality aids further optimization of TOPCon solar cell conversion efficiency.

## 2. Experimentals

The silicon wafers employed for the fabrication of TOPCon solar cells are of industrial grade, with a size of  $182\text{ mm} \times 182\text{ mm}$  in square and a thickness of  $\sim 150\text{ }\mu\text{m}$ , the structure of the adopted TOPCon solar cell is schematically shown in Fig. 1. These n-type substrates boast a resistivity range of  $0.5\text{--}2\text{ }\Omega\cdot\text{cm}$ . Subjecting all wafers to a sequence of standard cleaning and texturing etching procedures. Following by a series of critical processes to established selective boron emitters on the front side of the wafers: thermal boron diffusion, laser treatment, and post thermal oxidation, ensuring controlled sheet resistances of  $\sim 250\text{ }\Omega/\square$  in the light doped region and  $\sim 90\text{ }\Omega/\square$  in the heavy doped region. Following this step, the borosilicate glass layer was removed from the rear and edge of the wafer, leaving the front surface intact. Subsequently, the wafer underwent an alkali polishing process to remove the boron emitter on the rear and edge. On the polished surface, an ultra-thin tunneling oxide layer,  $\sim 1.5\text{ nm}$ , was generated through oxidation with  $\text{O}_2$  plasma. This was followed by the deposition of an in-situ phosphorus-doped amorphous silicon layer,  $\sim 115\text{ nm}$  thick, using an in-line magnetron sputtering system (JT8000 POPAID, Belightech). Phosphorus-doped silicon targets are used for phosphorus-doped a-Si deposition, and the plasma excited from Ar and  $\text{PH}_3$  precursor gases is introduced to increase phosphorus content, and the gas flow rate of Ar and  $\text{PH}_3$  can be independently controlled by three successively distributed zones. After

$860\text{ }^\circ\text{C}$ , 30 min thermal annealing at dry  $\text{N}_2$  environment, single-sided polysilicon passivating contact structure was formed on the rear [19].

After removing the borosilicate glass and phosphor-silicate glass from the surface of the wafer, the preparation of the anti-reflection passivation film on the front side starts with the deposition of a  $\sim 10\text{ nm}$   $\text{AlO}_x$  film by an in-line single side deposition atomic layer deposition (ALD) (Ideal Deposition Equipment & Applications Co., Ltd.), which is the most mainstream commercial TOPCon solar cell  $\text{AlO}_x$  deposition equipment available. Subsequently,  $\text{SiN}_x$ ,  $\text{SiO}_x\text{N}_y$  and  $\text{SiO}_x$  were sequentially deposited on  $\text{AlO}_x$  with a tubular PECVD equipment (M82300-12/UM, Red Solar Photoelectric Technology Co., Ltd.), and in order to further enhance the film formation quality of  $\text{AlO}_x$ , a  $\text{N}_2\text{O}$  plasma treatment (plasma oxidation, PO) was set up for 120 s prior to the start of the process, and the specific process setup is shown in Table 1. The process involves heating precursor gases, which is then excited by pulsed radio frequency to create a glow discharge, forming a plasma. Two corresponding graphite sheets are subjected to opposite alternating voltage, which accelerates the plasma to impact the gas between the plates. This action propels the plasma towards the surface of the silicon wafer, thereby completing the coating process. For the rear side, three layers of  $\text{SiN}_x$  with different refractive indices were deposited sequentially using a same type tubular PECVD, while plasma hydrogenation (PH) using  $\text{NH}_3$  as a precursor gas was performed prior to the deposition of each  $\text{SiN}_x$ , and the main processes are also listed in Table 1. Finally, the fabrication of TOPCon solar cells is completed by going through the standard screen printing and firing process.

The  $I$ - $V$  characteristics of the TOPCon solar cells are assessed using a solar simulator that replicates sunlight conditions. Quantum efficiency (QE, Enlitech) tester is used to assist in analyzing TOPCon solar cell performance. The evaluation of passivation quality for both the front and rear passivation film layers, both post-deposition and after the firing process, is conducted using implied open circuit voltage ( $iV_{oc}$ ). This parameter is obtained using Quasisteady-state photoconductance (QSSPC) measurements performed under 1-Sun equivalent light intensity with a Sinton WCT-120 lifetime tester [20]. An ellipsometry (EMPro-PV, ELLITOP) is used to monitor the refractive index and thickness variations of the deposited film. X-ray Photoelectron Spectroscopy (XPS) (Axis Ultra DLD, KRATOS) equipped with an Al  $K\alpha$  monochromatic X-ray source ( $h\nu = 1486.6\text{ eV}$ ) was utilized to compare the impact of plasma oxidation on the deposited  $\text{AlO}_x$  layers. Additionally, in order to evaluate the impact of plasma hydrogenation on the hydrogen content within the  $\text{SiN}_x$  layers, we utilized Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS 5 iontof, PHI NanoTOFII). This analysis employed a Cs + primary ion at 10 kV, with the sample set at a  $-5\text{ kV}$  potential to detect negative secondary ions. The analysis was performed with an impact energy of 15 kV.

## 3. Results and discussion

### 3.1. Plasma oxidation

The impact of the PO treatment on the properties of the  $\text{AlO}_x$  film is visually illustrated through the O 1s core level spectra within the X-ray Photoelectron Spectroscopy (XPS) results, as displayed in Fig. 2a. Prior to the peak fitting process, the Shirley background, accounting for inelastically scattered electrons, was eliminated. From the O 1s peak, peaks at  $\sim 530.8\text{ eV}$  and  $\sim 532.9\text{ eV}$  were meticulously deconvoluted. These correspond to the O–Al–O bands of  $\text{Al}_2\text{O}_3$  and Al–OH bands of Al(OH) $_3$ , respectively. We used the peak areas of the O–Al–O and Al–OH contributions within the O1s core levels to analysis the ratio changes of  $\text{Al}_2\text{O}_3$  to Al(OH) $_3$ . The band ratio is only 1.22 in  $\text{AlO}_x$  films that have undergone only the same thermal process without plasma treatment, whereas the application of plasma oxidation increases the ratio to 1.66 [21,22]. It stems from the design of our industrial in-line ALD system, which effectively balances capacity and cost considerations. In the system, the sample is conveyed on a transfer plate through the

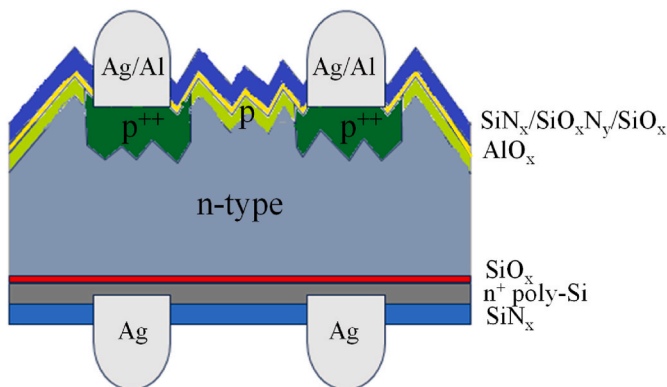
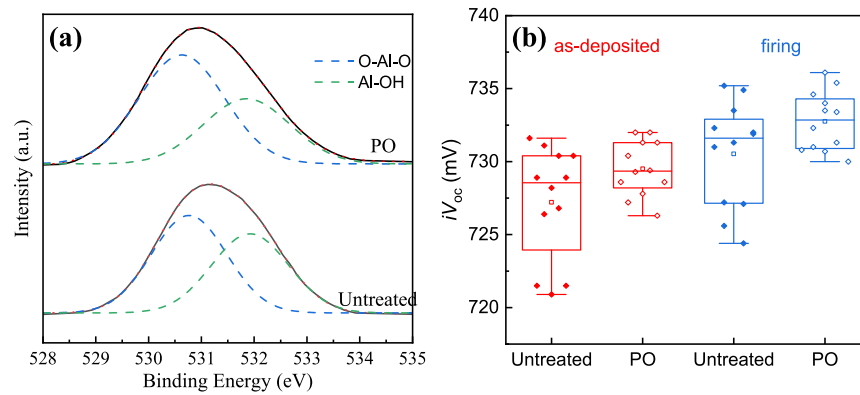


Fig. 1. Schematic diagram of the adopted commercial TOPCon solar cell structure.

**Table 1**

PO and PH process setting table for the front and rear film deposition process.

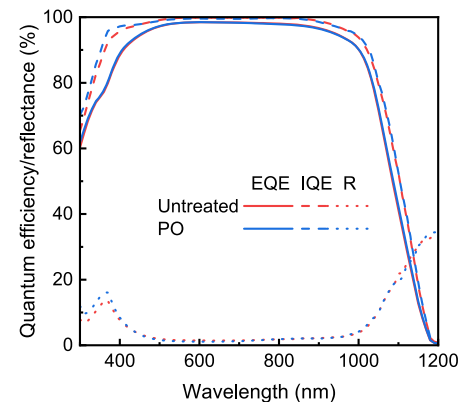
	Step	Time (s)	NH <sub>3</sub> flow (sccm)	SiH <sub>4</sub> flow (sccm)	N <sub>2</sub> O flow (sccm)	Power (W)	Pressure (mbar)
Front	Plasma oxidation	120	0	0	12,000	14,000	1650
	SiN <sub>x</sub> deposition	100	9335	2800	0	14,000	1650
		260	10,665	2000	0	15,500	1650
		180	10,655	1400	0	16,500	1650
	SiO <sub>x</sub> N <sub>y</sub> deposition	124	5200	1200	7400	14,400	1000
		144	5200	900	8935	14,400	1000
Rear	SiO <sub>x</sub> deposition	96	0	900	11,735	14,400	900
	Plasma hydrogenation	50	12,000	0	0	15,000	1800
	SiN <sub>x</sub> deposition	145	9800	2200	0	15,500	1800
	Plasma hydrogenation	50	16,000	0	0	15,500	1900
	SiN <sub>x</sub> deposition	180	14,000	2000	0	16,500	1900
	Plasma hydrogenation	50	15,200	0	0	15,500	1900
	SiN <sub>x</sub> deposition	390	14,400	1400	0	16,500	1900

**Fig. 2.** The change of AlO<sub>x</sub> XPS results at O 1s peak caused by PO treatment (a) and the effect on  $iV_{oc}$  values of final sample (b).

trimethylaluminum (TMA) and H<sub>2</sub>O chambers, undergoing recirculation until the desired thickness is achieved. However, the absence of stringent demarcation between the TMA and H<sub>2</sub>O regions gives rise to a less than optimal quality in the deposited AlO<sub>x</sub> film. It tends to harbor a significant quantity of oxygen vacancy defects and Al–OH bonds that fail to break in time, which remain intertwined due to their overlapping deposition processes. The integration of the PO process resulted in an elevation of the O–Al–O bond ratio, which can be attributed to the vigorous high-energy plasma bombardment, causing the rupture of O–H bonds. Consequently, the released Al and O from plasma reconfigure to form additional O–Al–O bonds, that aids in mitigating oxygen vacancy defects. Simultaneously, the liberated hydrogen from the fractured O–H bonds permeates into both the AlO<sub>x</sub> film and the AlO<sub>x</sub>/Si interface [23]. The collective impact plays a pivotal role in diminishing the density of defect states on the Si wafer surface. As a result, the effect of PO process on the values of the pre-metallization samples as shown in Fig. 2b. The PO process effectively improved the  $iV_{oc}$  values, and the average  $iV_{oc}$  values increased by more than 2 mV compared to untreated samples, both as-deposited and after firing, while at the same time the dispersion of the data distributions was much smaller, indicating that the homogeneity of the passivation had been significantly improved.

The final average electrical performance comparisons of TOPCon solar cells are shown in Table 2. The addition of extra PO treatment to the deposition process of the front surface passivation film helps the TOPCon solar cell to obtain an average  $V_{oc}$  gain of 1.3 mV. In addition,

the fill factor ( $FF$ ) is also obtaining a slight rise. There are two possible reasons for this, one is the higher  $V_{oc}$  due to better surface passivation quality which helps to increase the  $FF$ , and the other is that the PO treated AlO<sub>x</sub> film may be more easily penetrated by the metal paste to obtain lower contact resistivity. The overall effect on the cell conversion efficiency is an absolute average efficiency gain of 0.06%. The comparative analysis of QE and reflectance in Fig. 3 reveals that the PO treatment induces a marginal increase in reflectance within the 300–400 nm wavelength range. This change can be attributed to the slight alteration in the optical properties of the AlO<sub>x</sub> films resulting from the PO treatment. Specifically, the refractive index  $n$  of AlO<sub>x</sub> demonstrates a decrease from 1.63 to 1.60 by PO, as measured by ellipsometry. However, no significant effect on the AlO<sub>x</sub> thickness is observed following the PO treatment. Furthermore, the PO treatment has a

**Fig. 3.** Effect of PO treatment on the quantum efficiency of TOPCon solar cells.**Table 2**

Effect of PO treatment on electrical performance of TOPCon solar cells.

	Quantity	$V_{oc}$ (mV)	$I_{sc}$ (A)	$FF$ (%)	$\eta$ (%)
Untreated	1931	721.5	13.69	84.07	25.07
PO	1845	722.8	13.69	84.11	25.13

notably positive impact on the internal quantum efficiency (IQE) performance within the 300–400 nm wavelength range, due to the improved quality of the front surface passivation as shown in Fig. 2b. Nonetheless, the gain in external quantum efficiency (EQE) is not as apparent due to optical losses, which underscores the primary reason that the electrical performance enhancement resulting from the PO process primarily manifests in the  $V_{oc}$  gain, while any changes in  $I_{sc}$  are not readily discernible.

### 3.2. Plasma hydrogenation

The impact of PH treatment on the distribution of H atoms within both the  $\text{SiN}_x$  layer and the polysilicon passivating contact structure is elucidated through SIMS analysis, as showcased in Fig. 4a. Following the completion of  $\text{SiN}_x$  deposition, the PH treatment leads to a notable increase in H content within the deposited  $\text{SiN}_x$  layer can be measured, escalating from  $\sim 6 \times 10^{21}$  to  $\sim 1 \times 10^{22} \text{ cm}^{-3}$ . However, it exerts a lesser influence on the H content within the polysilicon layer as well as the tunneling oxide layer. Consequently, at this stage, PH treatment does not result in a significant change in passivation quality, as demonstrated in Fig. 4b. Upon subjecting the samples to the firing process, an essential step in the metallization of TOPCon solar cells, H atoms commence diffusion within the polysilicon passivating contacts and the underlying silicon substrate [24]. Notably, these H atoms accumulate near the interface  $\text{SiO}_x$ , consistent with findings reported in the literature [25]. In samples that underwent the PH process, the H content within the polysilicon and silicon substrate, particularly in the vicinity of  $\text{SiO}_x$ , is significantly higher compared to samples without PH treatment. This enrichment of H atoms near  $\text{SiO}_x$  proves beneficial as it contributes to a reduction in the density of unsaturated suspended bonds on the silicon surface. Moreover, the higher H content more effectively inhibits the passivation quality degradation of the passivating contacts during the firing process [13,26]. The outcome is evident in the samples subjected to PH treatment, displaying higher mean values of  $iV_{oc}$  ( $\sim 2.1 \text{ mV}$  higher than samples without PH treatment), accompanied by a reduction in the dispersion of  $iV_{oc}$  values, as shown in Fig. 4b. This clear trend underscores the pronounced effect of PH introduction in enhancing passivation quality.

In addition to enhancing passivation quality, PH treatment proves beneficial in elevating the overall electrical performance of TOPCon solar cells, as evidenced by the results presented in Table 3. The improvement in passivation quality contributes to a notable  $V_{oc}$  enhancement of approximately 1.1 mV. Importantly, there are no significant differences observed in the performance of  $I_{sc}$  and  $FF$ . This outcome aligns with the observation that PH treatment exerts minimal influence on the thickness and refractive index of the final  $\text{SiN}_x$  film, as determined by ellipsometry analysis. Finally, TOPCon solar cells achieve  $\sim 0.07\%$  average conversion efficiency gain by PH processing.

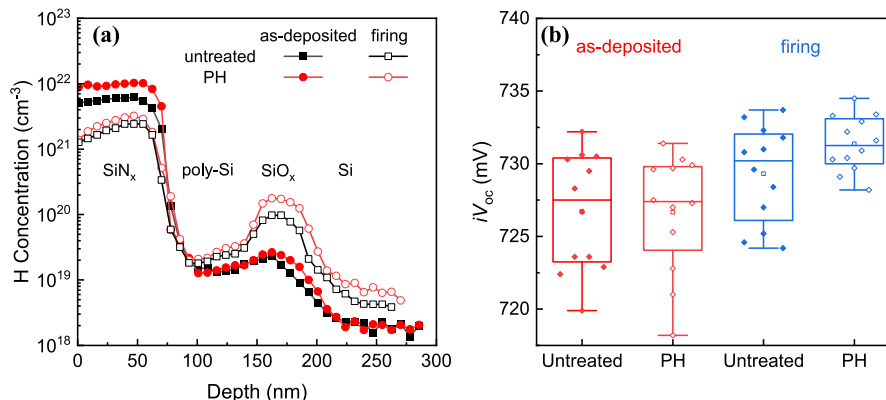


Fig. 4. Changes in H atom distribution caused by PH processing by SIMS extraction (a) and the effect on  $iV_{oc}$  values of final sample (b).

Table 3

Effect of PH treatment on electrical performance of TOPCon solar cells.

	Quantity	$V_{oc}$ (mV)	$I_{sc}$ (A)	$FF$ (%)	Eta (%)
Untreated	4368	722.8	13.66	84.04	25.05
PH	4889	723.9	13.68	84.02	25.12

### 4. Conclusions

In conclusion, our study has highlighted significant achievements in the optimization of TOPCon solar cells, with two key approaches on the anti-reflection passivation films. Firstly, for the front side film, we implemented a one-step PO process utilizing  $\text{N}_2\text{O}$  plasma. This process remarkably enhanced the quality of the in-line ALD-deposited  $\text{AlO}_x$  film by repairing the oxygen vacancy defects within it. The disruption of O–H bonds during this process additionally released H, contributing to passivation quality enhancement, evident by an impressive  $\sim 2 \text{ mV}$  increases in  $iV_{oc}$ , which ultimately resulted in a 0.06% improvement in efficiency. Furthermore, the application of the PH process prior to the deposition of each  $\text{SiN}_x$  layer on the rear side of the cell demonstrated compelling results. The SIMS analysis showed a significant increase in H content within  $\text{SiN}_x$  post-deposition. After the firing process, these H atoms diffuse towards the passivating contact and silicon substrate, becoming enriched in the  $\text{SiO}_x$  region. This enrichment effectively reduces the number of surface dangling bonds and helps inhibit the degradation of the passivating contact during firing. Consequently, the  $iV_{oc}$  value of the PH-treated sample demonstrated a substantial  $\sim 2.1 \text{ mV}$  increase compared to the untreated sample post-firing. This enhancement in the final electrical performance translated to an average efficiency gain of  $\sim 0.07\%$  for the TOPCon solar cells. The observed improvements in passivation quality and electrical performance demonstrate the potential of these optimization strategies in advancing TOPCon solar cell technology.

### CRediT authorship contribution statement

Wenhao Chen: Conceptualization. Shengxing Zhou: Investigation, Validation. Weiqing Liu: Investigation. Yingming Wang: Resources, Writing – review & editing. Penghui Chen: Investigation. Yuanyuan Yu: Investigation. Yimao Wan: Resources.

### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Data availability

Data will be made available on request.

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