Silicon Solar Cells



# Electron-Selective Scandium-Tunnel Oxide Passivated Contact for n-Type Silicon Solar Cells

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Dopant-free carrier-selective contacts have a high potential for cost reduction in solar panel production because of the simple structure and manufacturing procedure. Increasing the carrier selectivity is critical for improving the efficiency of heterostructure solar cells. Low work function metals have been explored as electron-selective contact (ESC) recently. In this paper, a highperformance silicon-oxide/scandium (SiOx/Sc) ESC structure is explored as an ESC that exhibits a good contact and surface passivation. The lowest contact resistivity of 23 m $\Omega$  cm<sup>2</sup> and the champion single-surface saturated dark current density ( $J_{oe}$ ) of 61 fA cm<sup>-2</sup> have been achieved with a full-area SiO<sub>x</sub>/Sc passivated contact. It was revealed that the ScO<sub>x</sub> formed by the reaction of Sc and SiO, was the critical material modifying the interfacial work function. Finally, the champion efficiency of >15% and an open circuit voltage ( $V_{oc}$ ) of >620 mV are achieved for the full-area rear SiO<sub>x</sub>/Sc passivated-contact n-type c-Si solar cell. A comprehensive analysis indicates that a high-efficiency n-type solar cell with efficiency of >20% is expected with the application of high-efficiency structures.

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## 1. Introduction

Doping-free heterojunction solar cell<sup>[1]</sup> has become a hot topic in photovoltaic as these devices avoid the traditional high-temperature diffusion process and the shortcomings brought by diffusion emitter, such as unwanted free carrier absorption and Auger recombination. Employing an n-type crystalline silicon wafer (c-Si) as the substrate for a doping-free heterojunction solar cell is a more reliable choice than p-type c-Si because of its relative insensitivity to transitional metal.

However, the block to develop the dopingfree n-type silicon solar cell is the direct metal contact with the lightly doped silicon, which typically exhibits Schottky characterization. To overcome this problem, the low work-function material,  $\text{LiF}_{x,}^{[1]}$  is introduced to serve as the high-efficiency electronselective-collection layer (ESCL) for an n-type c-Si solar cell. Nowadays, the doping-free n-type c-Si solar cell with low

work-function metals,  $[2^{-4}]$  oxides, [5-8] or fluorides[1,9] as the ESCL for high efficiency has been proven as an excellent structure, which lowers the contact resistivity to less than tens of m $\Omega \cdot \text{cm}^2$ . These results solve the long-term contact problem that impedes the development of high-efficiency n-type c-Si solar cell.

The application of a low work-function metal electrode for the rear contact displays a wider fabrication window than the dielectric materials, e.g., the oxides or fluorides. It does not need to control the thickness strictly because most of the low work-function metals are good conductors. The previous publications have demonstrated that magnesium  $(Mg)^{[3,10]}$  and calcium  $(Ca)^{[2,4]}$  have been successfully applied in the n-type c-Si solar cells with the efficiency of about 20%.

We considered that scandium (Sc) layer and an ultrathin tunnel oxide layer are the candidate ESCL for the passivated contact n-type c-Si solar cell due to the following advantages. First, to raise the selectivity of the carriers is of great importance to improve the efficiency of a solar cell.<sup>[11]</sup> Sc metal has a workfunction of about  $3.5 \,\text{eV}$ ,<sup>[12]</sup> which is lower than the workfunction of Mg ( $\approx 3.7 \,\text{eV}$ ), meaning that using Sc to replace Mg could achieve a smaller contact resistivity. Second, Sc should be chemically more stable than Ca. Because Ca is self-ignition in the atmosphere, while Sc is only oxidized in the atmosphere. Thus,



Sc is more suitable for a device, although Ca has a lower work-function of about 2.9 eV. Thus, in contrast with Ca, it is not necessary to deposit an Sc layer in a glove-box. Third, the tunnel oxide passivated contact structure, as one of the hottest topics,<sup>[13–23]</sup> has been proven its excellent surface passivation with the single-surface saturated dark current density ( $J_{oe}$ ) of <10 fA cm<sup>-2</sup>. Also, to deposit a tunnel oxide is much cheaper and flexible than the  $\alpha$ -Si:H thin film because of the avoidance of expensive PECVD system.

In this work, the Sc electron-selection electrode with passivated contact tunnel oxide (SiO<sub>2</sub>/Sc) was investigated thoroughly and was applied to the n-type c-Si solar cell. The interface structure, elemental distribution, interface workfunction, contact resistivity, and surface passivation of the SiO<sub>2</sub>/Sc contact were characterized. A contact resistivity ( $\rho_c$ ) of 23.5 m $\Omega$ -cm<sup>2</sup> and a low single-surface saturated dark current density ( $J_{oe}$ ) of 61 fA cm<sup>-2</sup> are achieved for the best SiO<sub>2</sub>/Sc ESCL, suggested that the n-type c-Si solar cell with the rear SiO<sub>2</sub>/Sc passivated contact has a potential efficiency of >20%.

#### 2. Experimental Section

The 4-inch n-type IC-grade Czochralski (CZ) c-Si wafers with a resistivity of 1–3  $\Omega$ -cm and a thickness of 270 nm were used as the substrates for the samples of contact resistivity and passivation effect measurements. The as-received wafers were first subjected to the alkaline etch to remove the sawing damage. A standard RCA clean with HF dip was adopted to remove surface contamination and native oxide. The thin oxide layer was grown in the 90 °C HNO<sub>3</sub> (68 at.%) bath for 4 min and then was subjected to the thermal treatments at 500-920 °C for 60 min with a high-purity N<sub>2</sub> atmosphere. An Sc layer of 15–20 nm was deposited using an electron beam evaporation (E-Beam) system with a 99.99% high-purity Sc pellets. Afterward, a capping layer of 800 nm aluminum (Al) was deposited on the Sc layer for the contact resistivity samples or a layer of 5 nm Al deposited on the Sc layer for the passivation samples. Such a thin Al layer is used to prevent the oxidation of Sc layer. Noted that the Al is deposited following the deposition of Sc without breaking the vacuum.

Solar-grade n-type CZ c-Si wafers with the (100)-orientation and a resistivity of 1–3  $\Omega$ -cm were used as the substrate for the solar cell fabrication. The random front pyramids were formed by KOH texturing and a 70  $\Omega$  sq<sup>-1</sup> p<sup>+</sup> emitter was realized by BBr<sub>3</sub> diffusion using a Tempress furnace. The front surface was passivated by a stack of PECVD Al<sub>2</sub>O<sub>3</sub> (about 12 nm) and SiN<sub>x</sub> (about 100 nm). Moreover, the previously mentioned SiO<sub>2</sub>/Sc structure was fabricated on the rear surface, followed by a thermal-evaporation of an Al capping layer of 1000 nm. The front metal-electrode pattern with a shading area of ≈8.7% was opened by photolithography and wet-chemical etch. Finally, the Ti/Pd/Ag electrode with a total thickness of 2 µm was deposited using electron beam evaporation and thermal-evaporation.

The passivation samples were examined using quasi-steadystate photoconductance (QSSPC) (Sinton WCT-120). The contact resistivity measurement was performed using a Keithley (4200-SCS) system. The thickness of tunnel oxide grown on polished CZ wafer is measured utilizing ellipsometer (J.A. Woollam, M-2000DI). The interfacial chemical bonding was characterized using the X-ray photoelectron spectroscopy (XPS) (AXIS ULTRA DLD). The work-function of the interfacial  $SiO_x/Sc$  was measured by ultraviolet photoelectron spectroscopy (UPS) (AXIS ULTRA DLD). The performances of solar cells are measured using an efficiency analysis system (Newport Oriel, SoliA) and a Suns-V<sub>oc</sub> analysis system (Sinton WCT-120). The quantum efficiency measurement is performed using a quantum analysis system (Newport Oriel, IQE200TM).

### 3. Results and Discussion

The structure of n-Si/SiOx/Sc(20 nm)/Al(800 nm) with various electrode pad diameters for the contact resistivity measurement is given in Figure 1a. To manifest the carrier-selective performance of the  $SiO_x/Sc$  ESC, the current-voltage (I-V) curves of n-Si/SiO<sub>x</sub>/Sc/Al and n-Si/Al are given for comparison. The oxides used in these structures are grown from nitric acid bath and then are subjected to one-hour under with high-purity N<sub>2</sub> atmosphere. The Al contact (the red lines) shows a rectifying I-V curve, indicating the Schottky contact. In comparison, most of the SiO<sub>x</sub>/Sc/Al contacts show the linear *I*–V curves expect the 920 °C-annealed oxide one, as given in Figure 1b. In another word, the SiO<sub>x</sub>/Sc/Al contact keeps as Ohmic contact with an oxide thickness of up to 2.7 nm that is corresponding to the 900 °C annealed oxide. However, the  $SiO_x/Sc/Al$  contact turns to a Schottky contact with a 3.0 nm oxide layer that is subjected to 920 °C annealing. In general, the SiO<sub>x</sub>/Sc/Al structure leads to improved carrier transportation in comparison with the SiO<sub>x</sub>/Al or SiO<sub>x</sub>/Mg/Al ESC,<sup>[10]</sup> as it can keep an Ohmic contact with a thicker oxide layer.

Cox-Strack method<sup>[24]</sup> is used to extract the contact resistivity through fitting the contact resistivity ( $\rho_c$ ) with the *I*–V curves obtained from different electrode pads. The extracted  $\rho_c s$  of the SiO<sub>x</sub>/Sc/Al contacts are given in Figure 1d. Noted that the  $\rho_c$  of Al contact cannot be extracted because of the rectifying *I*–V curve. In general, the  $\rho_c$  of the SiO<sub>x</sub>/Sc/Al contact is increased with the increase of annealing temperature, i.e., they are 23, 32, 47, 56, and 70 m $\Omega \cdot cm^2$  for the samples annealed at 500, 700, 800, 875, and 900 °C respectively. A contact resistivity of less than 100 m $\Omega \cdot cm^2$  is low enough for all rear-contact c-Si solar cells.

XPS and UPS measurements are carried out to identify the interfacial chemical bonding and the work functions to take a deep insight into the SiO<sub>x</sub>/Sc contact. Noted that the structure used for XPS measurement is n-Si/SiO<sub>x</sub>/Sc(20 nm)/Al(100 nm). The XPS spectra indicate that the interfacial Sc is oxidized significantly, as ScO<sub>x</sub> is dominated by the interfacial component (80%). The oxidized degree of Sc is much more significant than the one of Al, as shown in Figure 2a and b. The UPS measurement is carried out to identify the interfacial work function that is responsible for the improvement of carrier transportation by the application of Sc, as given in Figure 2c-e. Because of the oxidation, the ScO<sub>x</sub> should be the material that modifies the interfacial transport barrier. In this case, the Fermi level of Sc metal cannot be observed in the UPS spectra due to the oxidation. Instead of the Fermi level, the detectable signal in UPS is attributed to the electrons escaping from the top of the valence band of metallic oxides. Before extracting the electron energy from the valence band, it needs to identify the lowest





**Figure 1.** a) *I*–V curves of different pad areas on SiO<sub>x</sub> (875 °C)/Sc/Al stacks and the schematic diagram of the contact-measurement structure (inset). b) *I*–V curves of the SiO<sub>x</sub>/Sc/Al or SiO<sub>x</sub>/ Al contact with the oxide subjected to various annealing temperatures (the diameters of the pad dots are 3.6 mm). c) The oxide thicknesses and the corresponding annealed temperatures. d) Extracted contact resistivity of the SiO<sub>x</sub>/Sc/Al contacts.

kinetic energy (KE) point (originating from the secondary electrons of the equipment) and the highest KE point (originating from the electrons at the top of valence band). In this work, the low KE cut-off edge is determined by the intersection point of the two slopes of the KE curve, while the highest KE escaping energy is determined by the lowest point of the differential-treated KE curve, as indicated in Figure 2d and e. Finally, the SiO<sub>x</sub>/Sc interface exhibits a lower electron escaping WF of 0.65 eV than the SiO<sub>x</sub>/Al interface. Also, the electron escaping WF of SiOx/Sc contact is 0.15 eV lower than that of SiO<sub>x</sub>/Mg contact.<sup>[10]</sup> The differences of the electron escaping WF between the SiO<sub>x</sub>/Sc, SiO<sub>x</sub>/Al, and SiO<sub>x</sub>/Mg interfaces are generally consistent with the WF differences between the metal Sc ( $\approx$ 3.5 eV), Al ( $\approx$ 4.3 eV), and Mg ( $\approx$ 3.7 eV).

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**Figure 3**a–c show the cross-section images and elemental mappings of the c-Si/SiO<sub>x</sub>/Sc/ Al interface that is characterized using the high angle annular dark field scanning transmission electron microscopy (HAADF-STEM) and electron energy loss spectroscopy (EELS). The substrate c-Si is easily detected



**Figure 2.** a) XPS spectra of 2p for the AlO<sub>x</sub>. b) XPS spectra of 2p 3/2& 2p 1/2 for the ScO<sub>x</sub>. Note that in (a and b), the solid lines indicate the actual test results and the dotted lines represent the fitting spectrums. c) UPS spectra for the SiO<sub>x</sub>/Al and SiO<sub>x</sub>/Sc contacts. d) Local UPS spectra in zone 1. e) The detectable spectra in UPS of electron escaping WF from the top of valence band for the SiO<sub>x</sub>/Al and SiO<sub>x</sub>/Sc contacts (zone 2).



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Figure 3. a) TEM image, b) high-resolution TEM, and c) the EELS-mapping of the wafer/SiO<sub>x</sub>/Sc/Al interface.

due to its highly ordered crystalline nature. However, it is unexpected that we cannot find a SiO<sub>x</sub> interfacial layer in the TEM or HR-TEM cross-section images, although an annealed SiO<sub>x</sub> of about  $1.8 \pm 0.1$  nm was confirmed by ellipsometer measurement before the deposition of metal Sc. The layer of about 15 nm covered on the substrate c-Si is generally coincident with the thickness of the metal Sc layer deposited using E-Beam evaporation. The elemental distribution of the cross-section is carried out by EELS mapping to identify the interfacial chemical elements, as shown in Figure 3c. Three zones with different

element components are defined from the EELS mapping spectra: (I) Si, (II)  $ScO_x$ , and (III) Al (nm). Noted that the interfacial layer between the c-Si substrate and Al electrode was identified as  $ScO_x$  based on the detected Sc and O signals. The presence of  $ScO_x$  with the disappearance of  $SiO_x$  suggested the chemical reaction between Sc and  $SiO_x$ , which might be resulted from the high reactivity of Sc metal and the high inter-diffusivity between Sc and O.<sup>[25]</sup> The rest of oxygen may be originated from the oxygen trapped in the evaporation chamber and reacted with Sc and Al during the evaporation.

According to the table of activity series of metals, Sc is a kind of chemistry active metal, i.e., Sc can reactive with air or water. Generally,

Sc is much more active than Al metal. Loescher et al. have studied the oxidation of the metal Sc film with oxygen or air.<sup>[25]</sup> They found that the Sc film will be oxidized by oxygen at room temperature (23 °C) and that the ScO<sub>x</sub> film will grow to a thickness of 20 to 30 nm. The significant thickness of the ScO<sub>x</sub> layer also suggests the high chemical reaction between the Sc and oxygen and the great inter-diffusion between the Sc film and ScO<sub>x</sub> layer. It suggests that the ≈2.0-nm film has the capability of turning the ≈14-nm Sc layer into a ScO<sub>x</sub> film.



**Figure 4.** a)  $iV_{oc}$  and  $J_{oe}$  of the double-side passivated structure of Sc/SiO<sub>x</sub>/n-Si/SiO<sub>x</sub>/Sc. b) Effect of the oxide annealing temperature on the lifetime of the double-side passivated structure.

Table 1. Passivation of Al\_2O\_3/SiNx/ n-Si/SiN\_x/Al\_2O\_3 with annealing temperatures (minority carrier density is  $5\times10^{15}\,cm^{-3}).$ 

Temperature/°C	iV <sub>oc</sub> [mV]	$J_{\rm oe}$ [fA cm <sup>-2</sup> ]
w/o anneal	643	348
500	680	52
600	686	46
700	694	43.2
800	681	67.5
900	649	302

The passivation results of the double-side symmetrical Sc/SiO<sub>x</sub>/n-Si/SiO<sub>x</sub>/Sc structures, including surface saturated current density  $(I_{oe})$  and implied open circuit voltage (i $V_{oc}$ ), are given in Figure 4a. The oxide was grown at 90 °C in 68 at% HNO3 following thermal treatments at the temperatures ranging from 500 to 900 °C. The capping Sc layer is about 14 nm at each side to ensure the penetration of the flashing light. It is found that the as-grown oxide with the capping Sc shows no any surface passivation effect, which might be attributed to the significant interface defect density in the as-grown oxide. The SiO<sub>x</sub>/Sc starts to manifest surface passivation as if the oxide is subjected to thermal treatments. The Joe decreases gradually with the increase of annealing temperature, i.e., it is reduced from 2175 to  $61 \,\mathrm{fA} \,\mathrm{cm}^{-2}$  with the temperature increasing from 500 to 900 °C. It is encouraging that the champion  $I_{oe}$  of SiO<sub>x</sub>/Sc passivated contact is even better than the typical Joe of PERC passivated structure.<sup>[26]</sup> Different from the  $J_{oe}$ , the i $V_{oc}$  increases first but then decreases with the increase of temperature, leading to the champion  $iV_{oc}$  of  $\approx 630 \,\mathrm{mV}$  with the 700 °C annealed oxide, as shown in Figure 4a. The iVoc is not strictly corresponding with the  $J_{oe}$ , because the  $iV_{oc}$  is decided by both

the surface recombination and effective bulk lifetime. To illuminate this issue, the effect of annealing temperature on the effective lifetime is given in Figure 4b. The decrement of the lifetime was possibly due to the generation of thermal induced micro-defects, such as stack faults or impurity precipitation in bulk silicon, which leads to the decay of crystalline quality of the Si wafer.

The surface passivation of SiO<sub>x</sub>/Sc contact is attributed to both the thermal oxide and Sc layer. First, the thermal treatment helps the structural relaxation of silicon oxide, leading to a better bonding configuration with surface dangling bonds and a reduction of total interface state density ( $D_{it}$ ). The annealing at about 900 °C is helpful to eliminate the  $D_{it}$  of the interface. Second, the low work-function ScO<sub>x</sub> layer provides the field passivation effect, i.e., it leads to a downward bend of the energy band, reduces the accumulation of holes at the interface, and suppresses the carrier recombination.

Additionally, it is required to investigate the thermal stability of front-sided PECVD  $Al_2O_3/SiN_x$  stack layer before the fabrication of solar cell, since the  $Al_2O_3/SiN_x$  is also subjected to thermal treatment like the rear oxide layer. The n-type c-Si wafers covered with  $Al_2O_3/SiN_x$  on both sides are subjected to the one-hour thermal treatment ranging from 500 to 900 °C. The passivation is improved with the increment of annealing temperature from 500 to 700 °C, but it is impaired by the temperature of higher than 800°C. The deterioration of passivation is likely due to the SiN<sub>x</sub> that is not dense enough to withstand the high-temperature anneal. The best passivation of the annealed  $Al_2O_3/SiN_x$  is achieved with 700°C annealing, which leads to the champion  $J_{oe}$  of 40 fA cm<sup>-2</sup> and the champion i $V_{oc}$  of 694 mV, as given in **Table 1**.

We suggested that 700 °C is the optimal annealing temperature for oxides since good surface passivation is achieved by the front Al<sub>2</sub>O<sub>3</sub>/SiN<sub>x</sub> and rear SiO<sub>x</sub>/Sc contact simultaneously. In



**Figure 5.** a) Schematic device and b) energy band diagrams of the full rear-sided SiO<sub>x</sub>/Sc passivated-contact solar cell. c) The light J-V curves and d) EQE curves of the full rear-sided SiO<sub>x</sub>/Sc passivated contact and the full rear Al contact n-type c-Si solar cells.

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**Table 2.** Electrical parameters of devices obtained from the light J-V measurement.

Samples	V <sub>oc</sub> [mV]	$J_{\rm sc}~{\rm mA}\cdot{\rm cm}^{-2}$	FF [%]	Efficiency [%]
Full-area Al	583	31.37	57.3	10.5
	$583 \pm 4$	$31.2\pm0.3$	$56\pm 2$	$10.2\pm0.3$
SiO <sub>x</sub> /Sc	621	32.7	69.9	14.2
	$616\pm7$	$\textbf{31.8} \pm \textbf{1.1}$	$68.7 \pm 1.5$	$13.8\pm0.4$
Post anneal-250°C	620.5	32.30	75.5	15.1
	$620\pm2$	$31.5\pm0.8$	$75.2\pm0.3$	$14.9\pm0.2$
Post anneal-300°C	523	31.6	69.15	11.4
	$518\pm5$	$\textbf{31.8}\pm\textbf{0.3}$	$68.6 \pm 0.7$	$11.2\pm0.2$
Post anneal-350°C	455	31.3	69.56	9.9
	$449\pm8$	$31.1\pm0.4$	$69.2 \pm 1$	$9.5\pm0.4$

this work, the 700°C annealed SiO<sub>x</sub> is applied to the n-type solar cell. The structure and energy band diagrams of the full rearsided SiOx/Sc passivated-contact solar cell are given in Figure 5a and b. The best efficiency of 14.21% with an encouraging open-circuit voltage ( $V_{oc}$ ) of 621 mV, a short-circuit current  $(J_{sc})$  of 32.7 mA cm<sup>-2</sup>, and an enhanced fill-factor (*FF*) of 69.9% is obtained as the full rear-sided SiOx/Sc passivatedcontact solar cell with the 700 °C annealed oxide. The champion efficiency is coincident with the best passivation of the front and rear passivation layers. The controlled solar cell with full Al rearcontact exhibits the efficiency of 10.47% with a  $V_{\rm oc}$  of 583 mV, a  $J_{\rm sc}$  of 31.37 mA cm<sup>-2</sup>, and an *FF* of 57.3%. The improved efficiency is mainly from the improved  $V_{oc}$  and FF that benefit from the improved contact resistivity and surface passivation by the rear SiO<sub>x</sub>/Sc passivated contact. The external quantum efficiency (EQE) curves of both solar cells are given in Figure 5d. A significant improvement of quantum efficiency in the long wavelength range indicates better rear-sided passivation by the SiO<sub>x</sub>/Sc contact.

Furthermore, we investigated the effects of post-thermal anneal on performances of the rear  $SiO_x/Sc$  passivated-contact solar cell. The increment of the post-anneal temperature is helping to reduce the contact resistivity of  $SiO_x/Sc$  contact further, as indicated in **Figure 6**a, i.e., the slope of the *I*–*V* grows



**Figure 6.** a) *I*–V curves of the SiO<sub>x</sub>(700 °C)/Sc/Al contact with the post-RTP ranging 250–350 °C (the diameters of the pad dots are 3.6 mm). b) The light *J*–V curves of rear SiO<sub>x</sub>/Sc passivated-contact solar cells subjected to various post RTP annealing.

as the increment of post-annealing temperature up to  $350 \,^{\circ}$ C. The corresponding contact resistivity of 30, 27, and  $26 \,\mathrm{m}\Omega$ -cm<sup>2</sup> is observed with the post-annealing temperature at 250, 300,  $350 \,^{\circ}$ C, as shown in Figure 6b. Unfortunately, the passivation of SiO<sub>x</sub>/Sc contact starts to deteriorate as the post-annealing temperature exceeding 250 °C, which resulted in the decay of device's  $V_{\rm oc}$  and  $J_{\rm sc}$ , as shown in **Table 2**. An optimal post thermal treatment is essentially the trade-off between the *FF* and  $V_0/J_{\rm sc}$ .

The champion efficiency of 15.12% with a  $V_{oc}$  of 620.5 mV, a  $J_{sc}$  of 32.30 mA cm<sup>-2</sup>, and an *FF* of 75.47% is obtained with the 250 °C rapid thermal process (RTP) for 5 min, as shown in Figure 6b. The gain of efficiency is mainly originated from the improvement of *FF* by 5.6% in absolute value. According to the extracting from the light *I*–*V* and Suns- $V_{oc}$  measurements, the improved *FF* is mainly attributed to the reduction of series resistance ( $R_s$ ) from 3.1 to  $1.4 \Omega \cdot \text{cm}^2$ . The  $V_{oc}$  falls significantly as the temperature of the post-annealing is more than 300 °C, indicating the significant deterioration of the rear SiO<sub>x</sub>/Sc contact. Although the exact reason for this phenomenon is not revealed yet, we supposed that it was likely associated with the inter-diffusion of metal Sc, which induced significant interfacial defects through destroying the interface Si/SiO<sub>x</sub> bonding.

It is clear that the effect of SiO<sub>x</sub>/Sc on the rear surface passivation of n-type c-Si solar cells, but one may argue that the overall cell efficiency is still far from the state-of-the-art c-Si solar cells. Here we would like to discuss the reason for the low efficiency of the SiO<sub>x</sub>/Sc ESC solar cells, and we identify it is due to the non-optimized cell fabrication process. The main limiting factors for the efficiency include the fabrication compatibility, the optical reflectance, and the series resistance  $(R_s)$ , which lower the surface passivation, the  $J_{sc}$ , and *FF* respectively. In fact, for the SiO<sub>x</sub>/Sc contact, the best  $J_{oe}$  of about 60 fA cm<sup>-2</sup> and  $\rho_c$  of about 25 m $\Omega$ -cm<sup>2</sup> are quite good, which guarantees to fabricate a high-efficiency Si solar cell. If ignoring the above limiting factors by the poor fabrication and assuming the  $J_{\text{oe, rear SiOx/Sc}}$ ,  $J_{\text{oe, front}}$ ,  $J_{\text{oe, bulk}}$ ,  $J_{\text{oe, metal/Si}}$ ,  $J_{\text{sc}}$  and FF of an ideal SiO<sub>x</sub>/Sc ESC solar cell are 61 fA cm<sup>-2</sup>, 45 fA cm<sup>-2</sup>, 5 fA cm<sup>-2</sup>, 50 fA cm<sup>-2</sup>, 40 mA cm<sup>-2</sup>, and 80% respectively, the simulation efficiency of this solar cell is 21.66% with a  $V_{\rm oc}$  of 676 mV. In general, a Si solar cell with the SiO<sub>x</sub>/Sc ESC has the potential to achieve a high efficiency of >21.5%.

#### 4. Conclusion

In this paper, a novel structure of SiO<sub>x</sub>/Sc ESC Si solar cells is investigated, which exhibits an encouraging contact and passivation performances. Generally, the results of this work can be summarized as follows. (1) The SiO<sub>x</sub>/Sc structure shows excellent electron selectivity with a minimum contact resistivity of about 20 m $\Omega$ .cm<sup>2</sup>. The SiO<sub>x</sub>/Sc interface has a lower work function than the AlO<sub>x</sub> or the MgO<sub>x</sub> by 0.65 eV and 0.15 eV respectively. The SiO<sub>x</sub>/Sc contact can resist an oxide with a thickness of up to 2.7 nm. (2) ScO<sub>x</sub> is the certain material modifying the interface work function, which



is likely due to the chemical reaction between Sc and  $SiO_x$ . (3) The SiO<sub>x</sub>/Sc based contact shows excellent passivation for n-tye c-Si with a minimum  $I_{oe}$  of ~61 fA cm<sup>-2</sup>. (4) An optimal postthermal treatment is necessary for the further improvement of rear SiO<sub>x</sub>/Sc passivated-contact solar cell, although it is the tradeoff between the improvement of interfacial contact and the decay of surface passivation. (5) Finally, the champion efficiency of >15% with a V<sub>oc</sub> of >620 mV is achieved for the full-area rear SiO<sub>x</sub>/Sc passivated-contact n-type c-Si solar cell. A comprehensive analysis suggests that the efficiency of >20% is expected from the successful integration of high-efficiency structures.

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# **Conflict of Interest**

The authors declare no conflict of interest.

# **Keywords**

electron-selective contacts, low work function metals, scandium, tunnel oxide

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- [1] J. Bullock, M. Hettick, J. Geissbühler, A. J. Ong, T. Allen, C. M. Sutter-Fella, T. Chen, H. Ota, E. W. Schaler, S. D. Wolf, C. Ballif, A. Cuevas, A. Javey, Nat. Energy 2016, 1, 15031.
- [2] T. G. Allen, J. Bullock, Q. Jeangros, C. Samundsett, Y. Wan, J Cui, A H. Wyser, S. D. Wolf, A. Javey, A. Cuevas, Adv. Energy Mater. 2017, 7, 1602606.
- [3] Y. Wan, C. Samundsett, D. Yan, T. Allen, J. Peng, J. Cui, X. Zhang, J. Bullock, A. Cuevas, Appl. Phys. Lett. 2016, 109, 113901.
- [4] T. G. Allen, J. Bullock, P. Zheng, B. Vaughan, M. Barr, Y. Wan, C. Samundsett, D. Walter, A. Javey, Prog. Photovolt. Res. Appl. 2016, 25. 636.



- [5] X. Yang, P. Zheng, Q. Bi, K. Weber, Sol. Energy Mater. Sol. Cells 2016, 150, 32.
- [6] X. Yang, Q. Bi, H. Ali, K. Davis, W. V. Schoenfeld, K. Weber, Adv. Mater. 2016, 28, 5891.
- [7] J. He, Z. Ling, P. Gao, J. Ye, Solar RRL 2017, 1, 1700154.
- [8] Z. Ling, X. He, M. Liao, P. Liu, Z. Yang, J. Ye, P. Gao, IEEE J. Photovolt. 2017, 7, 1551.
- [9] Y. Wan, C. Samundsett, J. Bullock, T. Allen, M. Hettick, D. Yan, P. Zheng, X. Zhang, J. Cui, J. McKeon, A. Javey, A. Cuevas, ACS Appl. Mater. Interfaces 2016, 8, 14671.
- [10] H. Tong, Z. Yang, X. Wang, Z. Liu, Z. Chen, X. Ke, M. Sui, J. Tang, T. Yu, Z. Ge, Y. Zeng, P. Gao, J. Ye, Adv. Energy Mater. 2018, 1702921
- [11] Z. Yang, P. Gao, J. Sheng, H. Tong, C. Quan, X. Yang, K. W. A. Chee, B. Yan, Y. Zeng, J. Ye, Nano Energy 2018, 46, 133.
- [12] M. Hasan, H. Park, H. Yang, H. Hwang, H. Jung, J. Lee, Appl. Phys. Lett. 2007, 90, 34.
- [13] F. Feldmann, M. Bivour, C. Reichel, M. Hermle, S. W Glunz, A passivated rear contact for high-efficiency n-type silicon solar cells enabling high Vocs and FF> 82%. 28th European PV solar energy conference and exhibition, 2013.
- [14] Y. Zeng, H. Tong, C. Quan, L. Cai, Z. Yang, K. Chen, Z. Yuan, C. Wu, B. Yan, P. Gao, J. Ye, Sol. Energy 2017, 155, 654.
- [15] A. Richter, J. Benick, F. Feldmann, A. Fell, M. Hermle, S. W. Glunz, Sol. Energy Mater. Sol. Cells 2013, 173, 96.
- [16] F. Feldmann, C. Reichel, R. Müller, M. Hermle, Sol. Energy Mater. Sol. Cells 2017, 159, 265.
- [17] D. Yan, A. Cuevas, Y. Wan, J. Bullock, Sol. Energy Mater. Sol. Cells 2016, 152, 73.
- [18] Y. Tao, V. Upadhyaya, C Chen, A Payne, E. Lori. Chang, A. Upadhyaya, A. Rohatgi, Prog. Photovolt. 2016, 24, 830.
- [19] D. Yan, A. Cuevas, J. Bullock, Y. Wan, C. Samundsett, Sol. Energy Mater. Sol. Cells 2015, 142, 75.
- [20] A. Moldovan, F. Feldmann, M. Zimmer, J. Rentsch, J. Benick, M. Hermle, Sol. Energy Mater. Sol. Cells 2015, 142, 123.
- [21] F. Feldmann, M. Simon, M. Bivour, C. Reichel, M. Hermle, S.W. Glunz, Sol. Energy Mater. Sol. Cells 2014, 131, 100.
- [22] F. Feldmann, M. Bivour, C. Reichel, H. Steinkemper, M. Hermle, S.W. Glunz, Sol. Energy Mater. Sol. Cells 2014, 131, 46.
- [23] F. Feldmann, M. Bivour, C. Reichel, M. Hermle, S.W. Glunz, Sol. Energy Mater. Sol. Cells 2014, 120, 270.
- [24] R. H Cox, H. Strack, Solid-State Electron. 1967, 10, 1213.
- [25] D. H. Loescher, G. E. Pike, J. A. Borders, J. Vac. Sci. Technol. 1972, 9. 159.
- [26] A. Metz, D. Adler, S. Bagus, H. Blanke, M. Bothar, E. Brouwer, S. Dauwe, K. Dressler, R. Droessler, T. Droste, M. Fiedler, Y. Gassenbauer, T. Grahl, N. Hermert, W. Kuzminski, A. Lachowicz, T. Lauinger, N. Lenck, M. Manole, M. Martini, R. Messmer, C. Meyer, J. Moschner, K. Ramspeck, P. Roth, R. Schönfelder, B. Schum, J. Sticksel, K. Vaas, M. Volk,
  - K. Wangemann, Sol. Energy Mater. Sol. Cells 2014, 120, 417.