Effect of the front-metal work function on the performance of a-Si:H(n⁺)/a-Si:H(i)/c-Si(p) heterojunction solar cells

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Abstract

The present study investigates the effect of the front-metal work function on the energy band diagram and J – V characteristics under illumination of metal/a-Si:H(n⁺)/a-Si:H(i)/c-Si(p) heterojunction solar cells (HIT) by means of AFORS-Het device simulations supported by equivalent circuit modeling. It is found that for the heavily doped a-Si:H(n⁺) region, when the metal work function (φ_m) is not small enough to ensure a good ohmic contact ($3.9 \leq \varphi_m \leq 4.47$ eV), the observed decrease in the conversion efficiency (about 0.9%) with φ_m are due to the increase in the series resistance R_s . On the other hand, when φ_m exceeds 4.47 eV, the degradation of the open-circuit voltage V_{oc} (46 mV) and consequently the conversion efficiency η (about 3.3%) is related to the rectifying Schottky barrier at the metal/a-Si:H(n⁺) interface. Moreover, for moderately doped a-Si:H(n⁺) regions and large front-metal work function, the carrier recombination in the bulk increases significantly. The active electron density is reduced, and consequently, a strong enhancement of the dark current is observed which leads to a serious V_{oc} degradation. The J – V characteristics obtained from the circuit model analysis are in good agreement with the simulated results for different metal work functions.

Keywords Current–voltage characteristic · Series resistance · Reverse saturation current · Schottky barrier · Open-circuit voltage · Conversion efficiency

List of symbols

φ_m	Front-metal work function
D_m	Main diode
D_s	Schottky diode
V	Bias voltage
$V_m(V_s)$	Voltage across the main (Schottky) diode
$V_{m,s}$	Saturation voltage across the main diode
N_d	Doping level in the n ⁺ -region
$N_{d,act}$	Active electron density in the n ⁺ -region
$\phi_{b,eff}$	Effective Schottky barrier at the metal/a-Si:H(n ⁺) interface
J – V	Current–voltage characteristic
$J_{0m}(J_{0s})$	Reverse saturation current density of the main (Schottky) diode
J_{sch}	Schottky current density
J_{sc}	Short-circuit current density
V_{co}	Open-circuit voltage
η	Conversion efficiency

FF	Fill factor
$R_{sh}(r_{sh})$	Shunt resistance at the main (Schottky) diode
R_s	Series resistance

1 Introduction

The a-Si:H/c-Si heterojunction has been investigated as a promising candidate in many semiconductor device micro-electronic and photovoltaic applications. A lot of research work has been carried out for the last 30 years on amorphous/crystalline heterojunctions because of their application in photovoltaic field [1–11]. Although n-type wafers are usually used in commercial HIT solar cells, p-type c-Si wafer/substrates are attracting more attention by researchers due to lower material cost and popularity in the photovoltaic industry. Many research teams working on heterojunction solar cells have achieved over 20% conversion efficiency [12–14].

The a-Si:H/c-Si heterojunction solar cells with amorphous silicon intrinsic thin layer (HIT) are attractive as a high-efficiency, low-cost alternative to crystalline silicon (c-Si). Panasonic Corporation has reported that their HIT

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solar cells based on n-type c-Si currently have 24.7% conversion efficiency [15]. Owing to the large numbers of processing variables, such as the doping and the thickness of the emitter layer, the interface states density, the potential barrier creates in the back surface field, etc; it is a formidable task to scrutinize the effect of each physical parameter on the performance of the HIT solar cell experimentally. Nonetheless, a lot of simulations have been done to investigate the physical mechanism and the design optimization of HIT solar cells [16–18].

Hernandez-Como [17] displayed that the conversion efficiency of TCO/a-Si:H(p⁺)/a-Si:H(i)/c-Si(n)/a-Si:H(i)/a-Si:H(n⁺)/Al heterojunction solar cell, investigated by using the AMPS-1D software, is about 23% when the front contact is perfectly ohmic and the p/n interface is passivated. More recently, based on the AFORS-Het simulation program, Ghannam et al. showed that the open-circuit voltage and the conversion efficiency obtained from *J*–*V* characteristics of HIT solar cells on n-type c-Si substrate using TCO with adequate small work functions are degraded. This degradation has been explained by the Schottky barrier created at the TCO/a-Si:H(p⁺) interface [18].

The aim of this work is to study the effect of the Schottky barrier formed at the metal/a-Si:H(n⁺) front contact on the energy band diagram at equilibrium, the current–voltage characteristics and the photovoltaic parameters of the HIT cell. This study is based on the *J*–*V* results obtained from simulation with AFORS-Het devices of metal/a-Si:H(n⁺)/a-Si:H(i)/c-Si(p)/Al heterojunction solar cell for different front-metal work functions supported by the equivalent circuit modeling of two opposite polarity diodes in series.

2 Simulated results

Numerical simulation is now important for the understanding of the design and the optimization of heterojunction solar cells' high efficiency. Numerical simulation using AFORS-Het software shows that the front-metal contact nature has a great influence on the photovoltaic properties of heterojunction solar cells under one sun AM 1.5G.

The HIT structure to be simulated in the present study is sketched in Fig. 1 and consists of a 10-nm-thick n⁺-amorphous silicon layer (a-Si:H) realized on a 300 μm thick p-type crystalline silicon (c-Si) substrate with a doping concentration $N_d = 1.5 \times 10^{19} \text{ cm}^{-3}$ and $N_a = 10^{16} \text{ cm}^{-3}$, respectively. The a-Si:H(i) spacer (3 nm thick) is found essential for the high-quality passivation of the heterointerface [15]. The metal work function of the front contact varies in the range of 3.9–4.59 eV.

The current–voltage characteristics of the HIT cell with heavily doped a-Si:H(n⁺) layer under illumination, obtained by means of AFORS-Het simulation program for different

Fig. 1 Structure of the HIT cell under investigation

Fig. 2 Simulated current–voltage characteristics of the HIT cell, (a) under illumination and (b) in the dark

Table 1 Simulated photovoltaic parameters of metal/a-Si:H(n⁺)/a-Si:H(i)/c-Si(p)/Al heterojunction solar cell

φ_m (eV)	V_{oc} (mV)	J_{sc} (mA cm ⁻²)	FF (%)	η (%)
3.9	637.1	37.00	83.39	19.64
4.2	636.8	36.51	83.39	19.34
4.40	636.5	36.28	83.22	19.21
4.47	635.4	36.21	81.37	18.72
4.51	631.1	36.19	78.40	17.91
4.55	617.4	36.19	74.76	16.70
4.59	589.4	36.18	72.14	15.38

front-metal work functions (φ_m), are plotted in Fig. 2a. For values of φ_m smaller than 4.2 eV, the J - V characteristics under illumination have a quasi-normal shape predicted ($V_{oc} = 637$ mV and $J_{sc} = 37$ mA.cm⁻²). It is also observed that as the metal work function value exceeds 4.47 eV, the J - V curves are modified near the open-circuit voltage compared to the quasi-normal J - V characteristic. In Table 1, we have regrouped the photovoltaic parameters obtained for different values of φ_m . It is clear that the conversion efficiency of the HIT cell decreases about 4.2% when the metal work function value increases from 3.9 to 4.59 eV.

The simulated results of the dark J - V characteristics are plotted in Fig. 2b. From this figure, it is important to note that the dark current-voltage characteristic has an ideal form; i.e., the front contact is perfectly ohmic when the φ_m value is less than 4.2 eV. It can be concluded that the degradation in the conversion efficiency when φ_m value exceeds 4.2 eV is directly related to the dark current density since the illuminated current density ($J_{ph,m}$) is slightly reduced (about 0.8 mA cm⁻²) due to the barrier created at the metal/a-Si:H(n⁺) interface.

In the next section, using the J - V characteristics presented in Fig. 2a and b, we investigate the metal/a-Si:H(n⁺) interface based on a similar double-diode model and a straightforward technique that extracts the reverse saturation current densities of the two diodes, the series resistance and the effective barrier at the metal/a-Si:H(n⁺) interface.

3 Double-diode solar cell equivalent circuit

Taking into account the effect of the Schottky contact, Fig. 3 shows the circuit model of the HIT cell defined by two opposite polarity diodes in series. The main cell n⁺/p junction diode (D_m) and the Schottky diode (D_s) are connected by two current sources in parallel $J_{ph,m}$ and $J_{ph,s}$, respectively. The current density $J_{ph,m}$ refers to the total photocurrent density generated when the front contact is perfectly ohmic, whereas the second term represents the degradation of $J_{ph,m}$ when the metal work function is not low enough to ensure a good ohmic contact

Fig. 3 Equivalent circuit for double-diode model of the HIT cell under illumination

with the emitter layer. The equivalent circuit is completed by a series resistance R_s and two shunt resistances R_{sh} and r_{sh} which are connected in parallel to the D_m and D_s diodes, respectively. It is assumed that the circuit elements between points A and B and between B and C (see Fig. 3) can be treated as independent circuits.

Under illumination, the current-voltage characteristic between the points A and B can be expressed using Kirchhoff's laws as:

$$J = -J_{ph,m} + J_{0m} \left[\exp \left(\frac{qV_m}{nk_B T} \right) - 1 \right] + \frac{V_m}{R_{sh}} \quad (1)$$

where V_m is the voltage across the main diode, q is the electronic charge, k_B is the Boltzmann constant, and n is the ideality factor. T is the absolute temperature in kelvin. Neglecting the recombination of carriers in the space-charge region of the main junction n⁺/p, the ideality factor is equal to unity ($n = 1$).

The shunt resistance values are extracted from J - V characteristic in the dark at low polarization ($V \leq 0.25$ volts) by applying the Ohm's law:

$$V = J \times R_{sh} \quad (2)$$

In our study, the reverse saturation current density J_{0m} of the main junction diode is extracted when the J - V curve starts to show a rollover practically at $V_m = V_{m,s}$. Then, the J_{0m} values are extracted using this equation:

$$J_{0m} \simeq (J_{sc} + J) \times \exp \left(-\frac{qV_{m,s}}{nk_B T} \right) \quad (3)$$

J_{sc} is the short-circuit current density. It is practically the total photocurrent density of the equivalent circuit model ($J_{sc} = |J_{ph,m} - J_{ph,s}|$). According to Cheung-Cheung method [19], the series resistance can be extracted from J - V characteristic in the dark using:

$$\frac{dV}{d(\ln J)} = \frac{k_B T}{q} + R_s J \quad (4)$$

Since the emitter contact may induce a Schottky barrier at the metal/a-Si:H(n^+) interface, the current in the Schottky diode is governed by thermionic emission for $V \geq V_{m,s}$. Using the equivalent circuit between points B and C and neglecting the photocurrent $J_{ph,s}$, the Schottky current density (J_{sch}) is expressed as follows:

$$J_{sch} = -J_{0s} \left[\exp \left(\frac{qV_s}{k_B T} \right) - 1 \right] + \frac{V_s}{r_{sh}} \quad (5)$$

J_{0s} is the Schottky diode reverse saturation current density. It is the current density where the J – V curve starts to show a rollover, i.e., $J_{0s} \approx J(V = V_{m,s})$. It is given by:

$$J_{0s} = A^* T^2 \exp \left(-\frac{q\phi_{b,eff}}{k_B T} \right) \quad (6)$$

where A^* and $\phi_{b,eff}$ are the Richardson constant and the effective Schottky barrier at the metal/a-Si:H(n^+) interface, respectively. Away from the metal/a-Si:H(n^+) junction, the effective Schottky barrier is expressed by:

$$\phi_{b,eff} = \phi_m - \left(\chi - k_B T \ln \left(\frac{N_c}{N_{d,act}} \right) \right) \quad (7)$$

χ is the electronic affinity of amorphous silicon. N_c and $N_{d,act}$ are the effective states' density in the conduction band edge and the active electron density in the a-Si:H(n^+) layer, respectively. The voltage across the Schottky diode is given by:

$$V_s = V - V_m - JR_s \quad (8)$$

The values of the shunt resistance and the reverse saturation current density of the main diode calculated from Eqs. 2 and 3 are regrouped in Table 2. It should be noted that the J_{0m} values are practically constant when the ϕ_m value is less than 4.47 eV and undergoes a significant increase when the front-metal work function exceeds this value. This is explained by the increase in the Schottky barrier with increasing ϕ_m which is confirmed by the

simulated band diagrams at equilibrium displayed in Fig. 4. The decrease in the active electron density $N_{d,act}$ listed also in Table 2 is due to the interaction between the electric fields at the metal/a-Si:H(n^+) interface and at the a-Si:H(i)/c-Si(p) heterointerface, which results in a significant reduction in the free majority carriers in the a-Si:H(n^+) layer. Consequently, the reverse saturation current density in this region increases.

Using the dark current–voltage characteristics presented in Fig. 2b, the series resistance calculated from Eq. 4 increases sharply when the barrier at the metal/a-Si:H(n^+) interface is increased as depicted in Fig. 5.

Fig. 4 Simulated energy band diagram of the top 40 nm at equilibrium for different values of metal work function ($N_d = 1.5 \times 10^{19} \text{ cm}^{-3}$)

Fig. 5 Plots of the series resistance versus the metal work function

Table 2 Physical parameters calculated in our study for different ϕ_m values

ϕ_m (eV)	R_{sh} ($k\Omega \text{ cm}^2$)	J_{0m} (pA cm^{-2})	ΔV (sign)	$N_{d,act}$ (10^{19} cm^{-3})
3.9	28.74	0.750	> 0	1.5
4.2	28.71	0.752	> 0	1.5
4.40	28.10	0.752	> 0	1.49
4.47	27.80	0.798	~ 0	1.44
4.51	27.60	0.871	< 0	1.20
4.55	27.34	1.213	< 0	0.65
4.59	26.24	2.102	< 0	0.23

4 Analysis and interpretation of the cell performance under illumination

To better understand the effect of the series resistance and the Schottky barrier created at the front contact on the performance of the HIT cell, we introduce in our study the algebraic deviation between the saturation voltage $V_{m,s}$ and the open-circuit voltage V_{oc} given by:

$$\Delta V = V_{m,s} - V_{oc} \quad (9)$$

As mentioned earlier, the saturation voltage across the D_m diode is extracted from the simulated data of the J – V characteristic. Based on the ΔV signs extracted in our study (see Table 2), it can be also noted that the decrease in the conversion efficiency ($\sim 0.9\%$) when the value of ϕ_m increases from 3.9 to 4.47 eV is not related to the Schottky barrier as shown in Fig. 4. But it is due to the increase in the series resistance, since the $V_{m,s}$ value is large than the open-circuit voltage ($\Delta V \geq 0$).

On the other hand, when the front-metal work function values are greater than 4.47 eV, the main diode saturation voltage has a lower value than the open-circuit voltage ($\Delta V < 0$). Consequently, the 3.3% degradation of the conversion efficiency when ϕ_m value passes from 4.47 to 4.59 eV is due to the series resistance and the rectifying Schottky barrier at the front contact. Moreover, when the front-metal work function is larger than 4.47 eV, the active doping concentration in the n^+ -region decreases. The active electron density in the emitter layer at the heterointerface significantly drops leading to a strong enhancement of the reverse saturation current density J_{0m} and a serious V_{oc} degradation (about 46 mV) which results in a significant reduction in the conversion efficiency.

In Fig. 6, we showed the Schottky diode saturation current density versus the effective barrier created at the

Fig. 6 Schottky diode reverse saturation current density versus the effective Schottky barrier

metal/a-Si:H(n^+) interface. Generally, we observe that this variation follows a decreasing exponential law. The Richardson constant estimated from an exponential fit at room temperature is $116 \text{ A cm}^{-2} \text{ K}^{-2}$. This value is comparable to the one reported in the literature ($A^* = 120 \text{ A cm}^{-2} \text{ K}^{-2}$ for n -type semiconductor) [20].

The J – V characteristics of the HIT cell under illumination obtained by the circuit model analysis using the physical parameters listed in Table 2 are plotted in Fig. 7a for different metal work functions. The voltage drops across the different circuit elements determined from our analytical study are plotted in Fig. 7b as a function of the terminal cell voltage V . It should be noted from Fig. 7a and b that the effect of the series resistance on the J – V characteristic is dominant when the terminal cell voltage is less than the $V_{m,s}$ value. As the metal work function is increased, the Schottky current density saturates at a lower value, and hence, a rollover occurs at lower bias voltage. Note that the

Fig. 7 **a** Effect of the metal front contact on the J – V characteristics under illumination of the metal/a-Si:H(n^+)/a-Si:H(i)/c-Si(p) heterojunction solar cell ($4.47 \leq \phi_m \leq 4.59 \text{ eV}$). **b** Voltage drops across the different circuit elements as a function of the terminal cell voltage

Table 3 J_{0s} , R_s and r_{sh} values for different metal work functions

φ_m (eV)	J_{0s} (mA cm ⁻²)	R_s (Ω cm ²)	r_{sh} (Ω cm ²)
4.47	—	0.36	—
4.51	13.10	0.70	70
4.55	5.13	1.06	300
4.59	3.09	1.13	380

rollover changes dramatically over a relatively narrow range of φ_m ($\varphi_m > 4.47$ eV).

The effect of shunt resistance at the Schottky diode on rollover is also studied. The analytical results (Fig. 7a) showed that r_{sh} affects only the rollover part of the J – V curve ($V > V_{ms}$). The slope of the rollover curve is the leakage conductance at the front contact ($1/r_{sh}$). Hence, the fill factor is not affected by the magnitude of the shunt resistance (see Table 3).

As depicted in Fig. 7a, a good agreement is obtained between the simulated results and those of our circuit model analysis assuming a series resistance, Schottky saturation current density and a shunt resistance which are regrouped in Table 3. It is also important to note that the interpretations given in the previous paragraph concerning the degradation of the conversion efficiency and the open-circuit voltage as a function of the metal work function are confirmed by the J – V characteristics obtained from our circuit model analysis.

5 Effect of the doping level N_d on the performance of the HIT cell

The doping level of the a-Si:H(n^+) layer designates a physical parameter able to influence the Schottky barrier's height at the front-metal/a-Si:H(n^+) interface. For this reason, in this section, we study the effect of the doping level on the photovoltaic parameters of the HIT cell. Figure 8a and b shows the variation of the simulated open-circuit voltage and the conversion efficiency as a function of n^+ -layer doping level for different φ_m values.

As can be seen, the V_{oc} and the η values are practically not influenced by the doping level when the front contact is perfectly ohmic ($V_{oc} \sim 636$ mV and $\eta \sim 19.3\%$). It can be also noted that the performance of the HIT cell increases with the n^+ -layer doping when the metal work function is more than 4.2 eV.

The expanded view for the top 40 nm of the simulated energy band diagram at equilibrium of the HIT cell for moderately and heavily doped n^+ -layer ($N_d = 2 \times 10^{18}$ and 6×10^{19} cm⁻³) is presented in Fig. 9a and b, respectively. According to these band diagrams, it is important to note that the barrier's height at the metal/a-Si:H(n^+) interface for each φ_m value is identical for the two a-Si:H(n^+) doping

Fig. 8 **a** Open-circuit voltage of the HIT cell as a function of the a-Si:H(n^+) emitter doping level. **b** Conversion efficiency of the HIT cell as a function of the a-Si:H(n^+) emitter doping level

concentrations under study. On the other hand, when the emitter layer is moderately doped ($N_d = 2 \times 10^{18}$ cm⁻³), the separation between the conduction band and the Fermi energy in the quasi-neutral bulk region increases with the metal work function (see Fig. 9a). This is explained by the strong interaction between the electric fields at the metal/a-Si:H(n^+) and at the a-Si:H(i)/c-Si(p) interfaces. It can be concluded that the carrier recombination in the bulk of the emitter region increases, and the free electron density decreases. Consequently, the value of the shunt resistance decreases and the reverse saturation current density of the main diode is enhanced. Moreover, when the a-Si:H(n^+) layer is heavily doped, the interaction between the electric fields at the metal/a-Si:H(n^+) and at the a-Si:H(i)/c-Si(p) interfaces is very weak. The effect of the Schottky barrier on the reverse saturation current density of the main diode decreases.

Fig. 9 Simulated energy band diagram of the top 40 nm at equilibrium for different values of metal work function: **a** moderately doped n^+ -layer $N_d = 2 \times 10^{18} \text{ cm}^{-3}$ **b** heavily doped n^+ -layer $N_d = 6 \times 10^{19} \text{ cm}^{-3}$

Finally, compared to the perfectly ohmic metal/a-Si:H(n^+) interface ($\phi_m = 4.20 \text{ eV}$), Table 4 shows that for moderately doped n^+ -region the conversion efficiency and the open-circuit voltage undergo a significant degradation (about 4.5% and about 47 mV). The physical parameters of the equivalent circuit model (J_{0m} and R_{sh}) extracted in our study and regrouped in Table 4 confirm that the degradation of the

performance of the HIT cell is due to the decrease in the shunt resistance and the enhancement of the reverse saturation current density of the main diode when the Schottky barrier increases ($\phi_m \geq 4.48 \text{ eV}$).

6 Conclusion

The two-diode model simulation result helps to explain the effect of the Schottky barrier, created at the front contact, on the performance of metal/a-Si:H(n^+)/a-Si:H(i)/c-Si(p) heterojunction solar cells. This study is based on the current–voltage characteristics under one sun AM 1.5G established by AFORS-Het simulation program. This work illustrates that the open-circuit voltage and the J – V characteristics of the HIT cell with a large front-metal work function are degraded due to the Schottky barrier created at the metal/a-Si:H(n^+) interface.

The simulated band diagrams at equilibrium of the HIT cell show that the interaction between the electric field at the metal/a-Si:H(n^+) interface and the electric field at the a-Si:H(i)/c-Si(p) heterointerface is very weak. The Fermi energy in the quasi-neutral bulk a-Si:H(n^+) layer is close enough to the conduction band edge, where the emitter layer is heavily doped ($N_d > 10^{19} \text{ cm}^{-3}$). Moreover, if the emitter layer is moderately doped ($N_d = 2 \times 10^{18} \text{ cm}^{-3}$), the interaction between the electric fields is strong which results in a significant reduction in the free electron density in the a-Si:H(n^+) layer.

The J – V characteristics of the HIT cell under illumination obtained from the circuit model analysis show that, for heavily doped a-Si:H(n^+) region and when the metal work function is not small enough to ensure a good ohmic contact ($3.9 \leq \phi_m \leq 4.47 \text{ eV}$), the observed decreases in the conversion efficiency (about 0.9%) with ϕ_m are due to the increase in the series resistance. On the other hand, when ϕ_m exceeds 4.47 eV, the degradation of the open-circuit voltage (46 mV) and consequently the conversion efficiency (about 3.3%) is related to the rectifying Schottky barrier at the metal/a-Si:H(n^+) interface. Moreover, for moderately doped a-Si:H(n^+) region and large front-metal work function, the carrier recombination in the bulk increases significantly. The

Table 4 Photovoltaic parameters and the physical parameters of the metal/a-Si:H(n^+)/a-Si:H(i)/c-Si(p) heterojunction solar cell

$N_d \text{ (cm}^{-3}\text{)}$	$\phi_m \text{ (eV)}$	$V_{oc} \text{ (mV)}$	$J_{sc} \text{ (mA cm}^{-2}\text{)}$	FF (%)	$\eta \text{ (%)}$	$J_{0m} \text{ (pA cm}^{-2}\text{)}$	$R_{sh} \text{ (K}\Omega \text{ cm}^2\text{)}$
2×10^{18}	4.20	637.1	36.91	83.06	19.53	0.761	3.70
	4.48	631.1	36.64	75.95	17.56	1.932	2.45
	4.56	590.5	36.60	69.22	14.96	11.32	2.25
6×10^{19}	4.20	636.8	36.27	83.38	19.26	0.752	43.0
	4.48	635.9	36.26	81.37	18.76	0.754	42.8
	4.56	622.6	36.26	74.28	16.77	2.173	41.5

active electron density is reduced, and consequently, a strong enhancement of the dark current is observed which leads to a serious V_{oc} degradation. The J – V characteristics obtained from the circuit model analysis are in good agreement with the simulated results for different metal work functions.

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