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Numerical simulation of barrier height effect on output parameters, for a a-Si:H/nc-Si:H based solar cell

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Abstract. A numerical simulation by AMPS-1D (Analysis of Microelectronic and photonic structures) program has been carried out to examine the role of the front contact barrier heights φ_{b0} , ITO/P nanocrystalline layer contact, on the performances of a-Si:H n-i-p'-p solar cell with no back reflector. The p'-nc-Si:H buffer layer has been incorporated at the i/p interface in order to passivate the interface defects. Output parameters, like short circuit current (J_{SC}), open circuit voltage (V_{OC}), fill factor (FF) and efficiency (E_{ff}); for n-i-p'-p structure, are numerically simulated using different values φ_{b0}. The short circuit current is not very affected by φ_{b0}. However, for high values of φ_{b0} the other output cell parameters increase. The best values of V_{OC}, FF and Efficiency can be obtained for a value of φ_{b0} about 1.65 eV.

Keywords: numerical simulation, solar cell, a-Si:H silicon, ITO, barrier height.

1 Introduction

It is known that for hydrogenated amorphous silicon (a-Si:H) based solar cells, the quality of the p, i, and n layers can influence strongly the device performances. Another parameter which can affect these performances is the quality of the interfacial matching at the i/p interface and by the contacts to the doped layers as well [1]. It has been shown experimentally and with computer modelling, that hole barrier at the front contact/ p-layer interface can also influence hydrogenated amorphous silicon (a-Si:H) n-i-p solar cell performances [2]. In this report, we use the one-dimensional device simulation program AMPS-1D (Analysis of Microelectronic and Photonic Structure) to examine the role of front contact barrier heights φ_{b0} (ITO/p^+nc-Si:H contact) on the performances of n-i-p'-p solar cell with no back reflector. However, the device is amorphous (a-Si:H) and nanocrystalline (nc-Si:H) silicon based solar cell.

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2 Device modeling

2.1 About AMPS-1D

The modeling calculations uses the one-dimensional device simulation program for the Analysis of Microelectronic and Photonic Structures (AMPS-1D) developed by Fonash et al. at Pennsylvania State University, USA [3]. It estimates the steady-state band diagram, recombination profile, carrier transport in one dimension based on the Poisson equation and the electron and hole continuity equations. They are given respectively, by:

$$\frac{d}{dx}\left(-\varepsilon(x)\frac{d\Psi}{dx}\right) = q * [p(x) - n(x) + N_D^+(x) - N_A^-(x) + p_t(x) - n_t(x)] \quad (1)$$

$$\frac{1}{q}\left(\frac{dJ_n}{dx}\right) = -G_{op}(x) + R(x) \quad (2)$$

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$$\frac{1}{q}\left(\frac{dJ_p}{dx}\right) = -G_{op}(x) - R(x) \quad (3)$$

Where the electrostatic potential Ψ and the free electron n, free hole p, trapped electron n_t, and trapped hole p_t as well as the ionized donor-like N_D^+ and acceptor-like doping N_A^- concentrations are all functions of the position coordinate x. Here, ε is the permittivity and q is the magnitude of the charge of an electron. J_n and J_p are, respectively, the electron and hole current densities. The term R(x) is the net recombination rate resulting from direct band-to-band recombination and indirect Shockley-Read-Hall (SRH) recombination through gap states.
AMPS-1D provides two different approaches to the process of recombination and generation. One is the density of states (DOS), i.e., capture cross-section model. The other one is carrier lifetime model. In this work, we use the DOS model in the simulation of a-Si:H n-i-p solar cell based on hydrogenated amorphous silicon (for n and intrinsic layers) and hydrogenated nanocrystalline silicon for p and p' layers.

2.2 Structure of the simulated n-i-p'-p hetero-structure solar cell

For the simulation, we considered the amorphous a-Si:H based device, realized by Shiyong Liu et al [4]. The structures under study were fabricated by the radio frequency plasma enhanced chemical vapor deposition method (RF-PECVD). The device consists in a 300 nm thick amorphous and intrinsic a-Si:H layer, sandwiched between a 25 nm thick a-Si:H (n+) layer and a 15 nm thick p-type hydrogenated nanocrystalline nc-Si:H (p+) material, a 10 nm thick of p-type hydrogenated nanocystalline (p'-nc-Si:H) buffer layer, has been incorporated between the p+ and the intrinsic layer. (Fig.1).

The cell was grown on stainless steel substrate which plays the role of back contact. For the front contact, ITO electrodes were deposited, on the p+ side, using the RF sputtering technique, at 100°C.

3 Simulation results and discussion

3.1. Input parameters for simulation

The calculation, using the AMPS-1D program, requires the following input device parameters. The

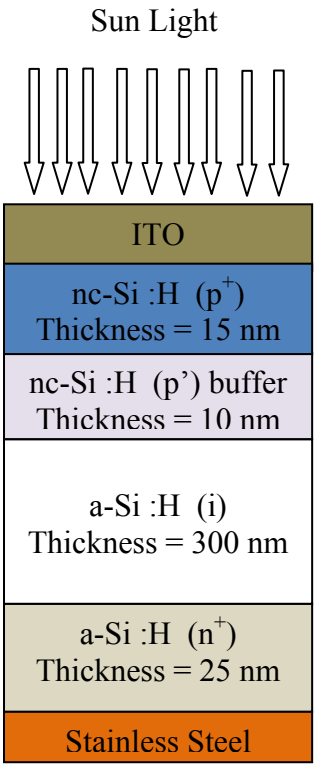

Fig.1. Schematic diagram of the amorphous/ nanocrystalline silicon hetero-junction

surface recombination velocities of both electrons and holes were set as 10^7 cm/s. In the model, in the thermodynamic equilibrium, at the front (x = 0) and back (x = L) contact, the barrier heights for electrons is specified as:

$$\varphi_{bo} = [E_C - E_F]_{x=0} \quad \text{and} \quad \varphi_{bL} = [E_C - E_F]_{x=L} \quad (4)$$

Here, E_c is the conduction band edge and E_f is the Fermi-level position in thermo dynamic equilibrium (see Fig.2). In this study, the barrier heights φ_{bo} at the front contact (ITO/p^+nc-Si:H) is taken to be 1.48 eV in all cases, except where the sensitivity to φ_{bo} is studied. At the back contact φ_{bL} (n^+-layer /SS) is taken to be 0.2 eV. φ_{bL} represents the activation energy of the n^+ layer. The n^+-layer doping is selected very carefully, which gives an activation energy for this n^+-layer material of E_a= 0.2 eV (see Table 1). This value agrees with the range of activation energy 0.2 eV reported for the n^+-layer material [5].

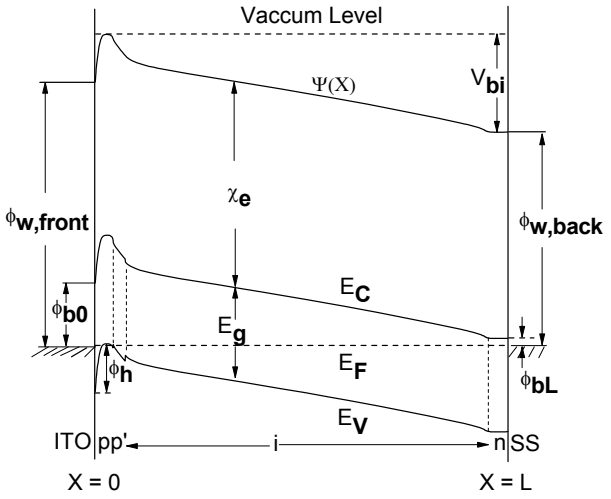

Fig.2. Band diagram of a n-i-p'-p hetero-junction solar cell structure in thermodynamic equilibrium.

A Solar AM 1.5 radiation with a power density of 100 mW/cm^2, as the illuminating source, was adopted. The light reflection at the front contact (RF) was set to 0.2. For the back contact and since there is no back reflector in the structure, we choosed 0 for back reflection (RB). For the intrinsic and n layers we choosed a value of 1.72 eV for the band gap energy E_g. All parameters described, in this section, and other used in the simulation are summarized in Table 1.

Table 1. Parameters extracted by simulating the experimentally measured solar cell characteristics of the n-i-p'-p a-Si:H/nc-Si:H structure. The abbreviations in table 1 are as follows: ε_r : Relative permittivity, L: Layer thickness, χ: Electron affinity, E_g: Band gap, E_a: Activation energy, N_C: Effective conduction band density, N_V: Effective valence band density, μ_{e^-}: Electron mobility, μ_{h^+} : Hole mobility, N_A: Acceptor doping, N_D: Donor doping, G_{DO}/G_{AO} : Exponential prefactors of donor-like or acceptor-like tail states, E_D/E_A: Characteristic energy of the donor-like /acceptor-like tail states, , N_{DG}/N_{AG} : Gaussian density for donor and acceptor states, E_{DG}/E_{AG} (eV) Donor and Acceptor Gaussian peak energy position.

Parameters	nc-Si:H(p^+)	buffer layer nc-Si:H(p')	a-Si:H(i)	a-Si:H(n^+)
ε_r	11.9	11.9	11.9	11.9
L (nm)	15	10	300	25
χ (eV)	3.70	3.75	3.8	3.8
E_g (eV)	2.0	1.88	1.72	1.72
E_a (eV)	0.06	0.07	0.8	0. 2
N_C (cm^{-3})	2.80 x 10^{19}	2.80 x 10^{19}	2.50 x 10^{20}	2.50 x 10^{20}
N_V (cm^{-3})	1.04 x 10^{19}	1.04 x 10^{19}	2.50 x 10^{20}	2.50 x 10^{20}
μ_{e^-} (cm^{2}V^{-1}s^{-1})	2.0	2.0	20	10
μ_{h^+}(cm^{2}V^{-1}s^{-1})	0.2	0.2	2.0	10
N_A (cm^{-3})	3 x 10^{19}	1 x 10^{16}	0	0
N_D (cm^{-3})	0	0	0	1 x 10^{19}
G_{DO}/G_{AO}(cm^{-3}eV^{-1})	2 x 10^{20}	2 x 10^{20}	2 x 10^{21}	2 x 10^{21}
E_D/E_A (eV)	0.06 / 0.01	0.06 / 0.01	0.05 / 0.03	0.05 / 0.03
σ_{de} (cm^2) (Tails)	1 x 10^{-15}	1 x 10^{-15}	1 x 10^{-15}	1 x 10^{-15}
σ_{dh} (cm^2) (Tails)	1 x 10^{-17}	1 x 10^{-17}	1 x 10^{-17}	1 x 10^{-17}
σ_{ae} (cm^2) (Tails)	1 x 10^{-17}	1 x 10^{-17}	1 x 10^{-17}	1 x 10^{-17}
σ_{ah} (cm^2) (Tails)	1 x 10^{-15}	1 x 10^{-15}	1 x 10^{-15}	1x10^{-15}
N_{DG} (cm^{-3})	1 x 10^{17}	1 x 10^{16}	5 x 10^{15}	5 x 10^{18}
N_{AG} (cm^{-3})	1 x 10^{17}	1 x 10^{16}	5 x 10^{15}	5 x 10^{18}
E_{DG} / E_{AG} (eV)	1.50 / 0.98	1.38 / 0.78	1.22 / 0.70	1.22 / 0.70

3.2. Results and discussion

In the past works and surprisingly, it was found that, for front contact barrier height values φ_{b0} less than some critical value, cell performances, in the absence of tunneling, depends strongly on the front contact barrier height regardless of the thickness or the quality of the p-layer [6, 7]. In AMPS, barriers at ITO/p interface and n/metal interface are described by φ_{b0} and φ_{bL} respectively. The barrier heights φ_{b0} and φ_{bL} are depicted in Fig. 2, which shows the band diagram of a n-i-p'-p hetero-junction solar cell structure in thermodynamic equilibrium. According to J. Arch et al. [6] description the barrier heights are related to the work functions ($\Phi_{w,front}$ and $\Phi_{w,back}$) of the contacts by:

$$\varphi_{b0} = \Phi_{w,front} - \chi_e|_{x=0} \quad (5)$$

$$\varphi_{bL} = \Phi_{w,back} - \chi_e|_{x=L} \quad (6)$$

Where χ_e is the electron affinity (see Fig. 2).

The quantity φ_h in Fig. 2 denotes the amount of band bending at thermodynamic equilibrium in the p^+nc-Si:H material; it depends on the front contact metal (ITO in this case) i.e., the value of φ_{b0}, the p^+ layer doping and the density of state (DOS), and the thickness of the p-layer. However, if the p-layer is sufficiently thick, then the value of φ_h will only depend on the value of φ_{b0} and on the p-layer doping and DOS, and can given by:

$$\varphi_h = \varphi_{b0}^{\,n} - \varphi_{b0} \quad (7)$$

Where $\varphi_{b0}^{\,n}$ is the barrier height value, for a given p-layer doping that would give a neutral (no band bending φ_h= 0 eV) contact to the p-layer material. From Eq. (7) can see that smaller values of φ_{b0} will give larger values of φ_h. Since holes are collected at the front contact, this band bending φ_h presents a barrier to photogenerated holes trying to exit the cell. In this numerical simulation study, we take φ_{b0} to be in the range of 1.15-1.85 eV. If the p^+nc-Si:H is sufficiently thick (15 nm in our case, see Fig. 1), these barrier height values result in band bending φ_h for holes near the front contact (see Fig. 2) that varies from φ_h = 0 (for $\varphi_{b0} = \varphi_{b0}^{\,n}$ = 1.85 eV) to φ_h = 0.7 eV (for φ_{b0} = 1.15 eV).

Figure 3 shows an important improvement in the external parameters of the n-i-p'-p solar cell and this result is mainly due to the increase of the barrier height φ_{b0}. When φ_{b0} increases form 1.15 eV to 1.85 eV, the values of the whole barrier height φ_h decreases from 0.7 eV to 0 eV. This facilitates the collection of the photogenerated holes at front contact side of the cell.

According to Equation (5) and results, showed in Figure 3, the critical value of φ_{b0}, for which solar cells performances are reduced and which corresponds to a value of 0.2 eV for φ_h, is 1.65 eV. This value of φ_{b0} can be obtained experimentally by an optimal value of the work function of the ITO ($\Phi_{w,front}$), about 5.35 eV. The ITO work function can vary from 4.3 to 5.3 eV, depending on the stochiometry and the deposition method of ITO layer [8]. In particular, the work function of ITO was modified by a self-assembled monolayer (SAM) and a value of 5.695 eV was obtained [9,10].

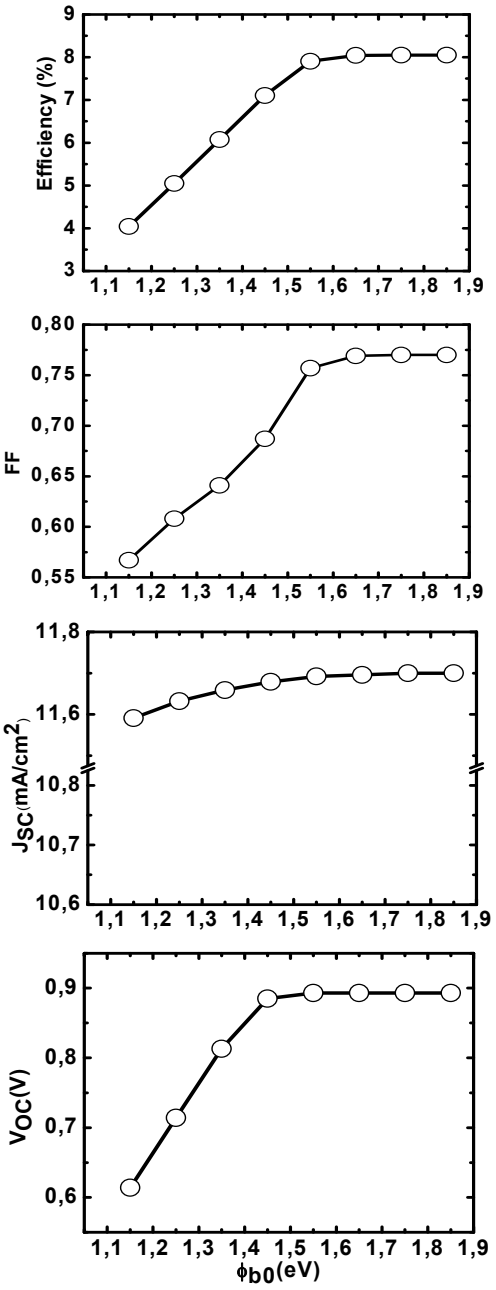

Fig. 3. Effect of front contact barrier height (φ_{b0}) on n-i-p'-p solar cell output parameters.

Finally, in Table 2, we compare our simulation results to the experimental data obtained by Shiyon Liu [4], on the structure n-i-p'-p with a buffer layer. Firstly, for the value of φ_{b0} = 1.48 eV, a good agreement can be seen between our simulation results and experimental data. This agreement confirms the validity of the input parameters summarized in Table 1. Secondly, the best cell's external parameters can be obtained with a value of 1.65 eV for φ_{b0}.

Table 2 . Comparison between experimental and modeled solar cells output parameters for the n-i-p'-p structure

Reference	V_{OC} (V)	J_{SC} (mA/cm^2)	FF	E_{ff} (%)
Experimental Results [8]	0.896	11.710	0.709	7.44
This work φ_{b0} = 1.48 eV φ_{b0} = 1.65 eV	0.890 0.893	11.684 11.696	0.712 0.769	7.40 8.04

Conclusion

In this study, AMPS-1D software code has been used to simulate a silicon n-i-p'-p solar cells with no back reflector. Our objective was to study the influence of the barrier height for electrons (φ_{b0}) or holes (φ_h), at ITO/p^+ front contact, on the solar cell performances. The simulation allowed us to extract some important and realistic parameters, characterizing each layer of the structure wich was recently realized. The modelling showed that for p^+ and n^+ layers, sufficiently thick and sufficiently doped, the reverse bias currents, both in the dark and under illumination, do not depend on the front contact barrier heights. However, in the forward direction, this contact barrier influences strongly, both the dark and illuminated currents. The best results obtained for the short circuit current (J_{SC}), the open circuit voltage (V_{OC}), the fill factor (FF) and the efficiency (E_{ff}) were obtained when the barrier height value of φ_{b0} is about 1.65 eV. The value of efficiency, obtained by Shiyon Liu et al. is 7.44 % and corresponds to electron barrier height (φ_{b0}) about 1.48 eV used in our simulation. The efficiency can be really increased to a value of 8.04 %, if an ITO layer with a work function of 5.35 eV is deposited on the p^+ layer. This situation is experimentally realizable since higher work function value, about 5.695 eV, was already obtained by other deposition techniques.

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