Modelling and Computer Of The Band Bending In Heterojunction With Intrinsic Thin Layer Solar Cells.

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ABSTRACT

Among the factors limiting the open circuit voltage of Heterojunctions with Intrinsic Thin layers "HIT" solar cell, the surface potential barrier at the Indium Tin Oxide (ITO)/hydrogenated amorphous silicon (a-Si:H) interface is one of the most important. To reduce this surface potential barrier, we have varied the band bending by simulation. The aim is to understand why, in spite of a considerable change in the front contact barrier height at the interface ITO/n-a-Si:H (band banding reduced), the characteristics J(V) remain almost unchanged.

Keywords: Simulation; HIT solar cells; potential barrier; band bending; Current-voltage J(V) characteristics.

1. INTRODUCTION

The HIT Structure (Heterojunctions with Intrinsic Thin layers) created by the SANYO research group has a principal advantage compared to conventional solar cells : the use of hydrogenated amorphous silicon (a-Si:H) to produce both the emitter and back layers at low temperature (200°C) compared to the high temperature (1000°C) deposited technology of crystalline silicone (c-Si) cells. Indeed, p and n-type substrates are recently under intensive investigations since they are combining the low cost and low temperature process of hydrogenated amorphous silicon (a-Si:H) deposition coupled with the high efficiency and high stability of crystalline silicone (c-Si). An important scientific and technological progress on HIT structures has led to solar cells with efficiencies up to 21% [1, 2].

In spite of this progress, the solar cell efficiency is greatly limited by the recombination at the Transparent Conductive Oxides TCO/a-Si:H interface. TCO: Tin Oxide (S_nO_2) and Indium Tin Oxide (ITO) deposited on glass are widely used as window layer in the fabrication of a-Si:H based solar cells because of their low sheet resistance and high transparency in the visible region. However, many problems are associated with the use of these transparent conductive oxides. It is thus necessary to reduce the ohmic and optical losses generated by this interface.

It has been shown that it is possible to form a good Schottky diode between TCO and a-Si:H without a decrease of optical transmission if we interpose a thin Palladium or Chrome film [3,4]. In agreement with these experimental results, computer models on the effects of the height of the front contact barrier have shown that the front barrier ϕ_{b0} has to be increased (band-banding reduced) to increase the efficiency of a HIT n-type c-Si substrates: Indium Tin Oxide (ITO)/p-doped hydrogenated amorphous silicon (p-a-Si:H)/i-polymorphous (pm-a-Si:H)/n-doped crystalline silicon (n-c-

Si)/Aluminum (Al). Indeed, a remarkable improvement on Voc and FF has been achieved with the improvement of ϕ_{b0} [5]. This augmentation is due to the reduction of the surface potential barrier (seen by holes) which occurs at the interface. A reduction of this surface potential barrier leads to an augmentation of built-in potential V_{bi} and consequently an increase of V_{oc}. The reduction of the field at the ITO/p-layer interface will support the passage of the holes towards ITO. A large improvement of FF has been obtained because of the reduced interface recombination between ITO and p-layer [5].

The device used in the present work consists of a HIT p-type c-Si substrates (ITO/n-a-Si:H/i-pm-Si:H/p-c-Si/Al) Figure 1.

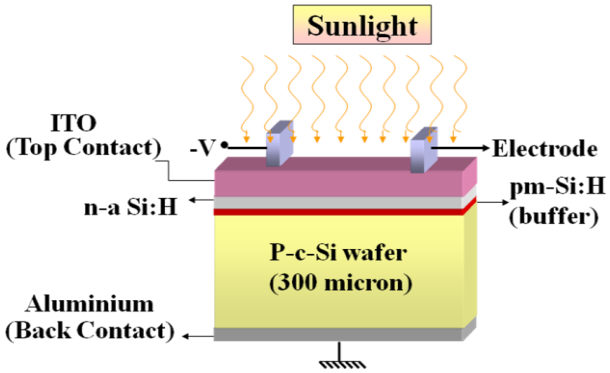

Figure 1: Schematic diagram of a HIT p-type c-Si substrates (ITO/n-a-Si:H/i-pm-Si:H/p-c-Si/Al) Solar Cell

For light through the n layer ϕ_{b0}, χ_0 represent the contact barrier height and the electron affinity of the n-a-Si:H layer, while ϕ_{bL} , χ_L are those of p-c-Si. V is the applied forward biased potential. The contact barrier heights between the n-layer and ITO at x =0 (ITO/n-a-Si:H figure 6) is given by:

$$\phi_{b0} = E_{ac}(n) \pm E_{sbb} \qquad (1)$$

And at the back contact, the barrier heights ϕ_{bL} between the p-layer and aluminum at x=L (p-c-Si/Al), is given by:

$$\phi_{bL} = E_g - E_{ac}(p) - E_{sbb}' \qquad (2)$$

E_{sbb} is the band bending at the front contact (ITO/n-a-Si:H). At the back contact (p-c-Si/Al), E_{sbb}' is taken equal to zero. These contacts are characterized by surface recombination speeds for each carrier (taken here to be S_{n0}, S_{p0}, S_{nL} and $S_{pL} = 10^7$ cm/sec for holes and electrons). $E_{ac}(n)$ et $E_{ac}(p)$ are the activation energy of the n and p layers. The barrier height ϕ_{b0} at the front contact ($\boldsymbol{x} = 0$) is depicted in figure 6, which shows this contact in a solar cell structure in thermodynamic equilibrium. This barrier height value and the other important parameters that we use in these simulations are listed in table 1.

Parameters	n-a-Si :H	i-pm-Si :H	p-c-Si
d (A°)	80	30	300 x10^4
χ (eV)	4.00	3.95	4.22
E_μ (eV)	1.80	1.96	1.12
E_{ac} (eV)	0.21	0.92	0.06
ND, NATOT (cm^{-3})	9.0x10^{18}	1.0x10^{14}	4.0x10^{18}
E_D (eV)	0.050	0.050	0.005
E_A (eV)	0.030	0.030	0.003

G_{D0}, G_{A0} (cm^{-3} eV^{-1})	$4.0x10^{21}$	$4.0x10^{21}$	$4.0x10^{20}$
μ_n (cm^2/V s)	20	30	1000
μ_p (cm^2/V s)	4	12	450
ϕ_{b0} (eV)	0.12-0.28		
ϕ_{bL} (eV)	1.06		

Table 1: Principal input parameters

In order to simulate and study the effect of the surface band bending E_{sbb} (the ITO/n-surface band bending) we have varied this band bending by changing the E_{sbb} in order to improve the ohmic contact between the ITO and n-layer fig4.

We chose the polymorphous silicon as an intrinsic thin layer because of its excellent electric properties [6]. The principal parameters of polymorphous silicon compared to amorphous silicon are summarized in table 2.

Result	Reference:
Density of states smaller in pm-Si:H than in a-Si:H. At room temperature electronic mobility-lifetime product up to a factor 200 higher in pm-Si:H than in a-Si:H	C. Longeaud et al [7]
Midgap density of states of pm-Si:H at least ten times lower than in a-Si:H Electron capture cross-section of deep gap states lower in pm-Si:H by a factor of 3-4	M. Meaudre et al. [8] J.P. Kleider et al. [9]
Faster kinetics of creation of metastable defects and better properties in both as-deposited and light-soaked states for materials with improved range order (pm-Si:H and c-Si:H)	P. St'ahel et al. [10]
Mobility of holes of 0.08 $cm^2.V^{-1}.s^{-1}$ in pm-Si:H and 0.010 $cm^2.V^{-1}.s^{-1}$ in a-Si:H	R. Brenot [11]
Excellent stability during light-soaking and a efficiency close to 10%	Roca i Cabarrocas et al. [12,13]

Table 2: The main parameters of polymorphous silicon compared to amorphous silicon.

2. SIMULATION MODEL

We have used ASDMP simulation model (Amorphous Semiconductor Device Modeling Program) developed by the group of professor Parsathi Chatterjee [14]. Prof. Roca's group at École polytechnique de Paris, France, has demonstrated experimentally that ASDMP model mimics the performance of p-i-n and HIT solar [15].

ASDMP examines the behaviour of semiconductor device structures under steady state in one dimension by solving simultaneously Poisson's equation, the continuity equations for free electrons and the continuity equation for free holes using finite differences and the Newton-Raphson technique, and yields the J(V) characteristics and the quantum efficiency. These equations are:

$$\frac{d}{dx}\left(\varepsilon(x)\frac{d\psi(x)}{dx}\right)=\rho(x). \quad (3)$$

$$0=\frac{1}{q}\frac{dJ_n(x)}{dx}+G_{opt}(x)-R_{net}(x). \quad (4)$$

$$0=\frac{1}{q}\frac{dJ_p(x)}{dx}+G_{opt}(x)-R_{net}(x). \quad (5)$$

In Poisson's equation "Eq. (3)", ε(x) is the dielectric permittivity of the semiconductor. Ψ(x) is the potential energy of an electron at the vacuum level in electron volts, and ρ(x) is the space charge density in the semiconductor. In the continuity equations "Eq. (4)-(5)", J_n (x) and J_p (x) are the electron and hole current, respectively, and *q* is the charge of electron. The term G_{net} ***(x)*** represents the net optical generation of free electron-hole pairs per unit volume, while R_{net} (x) denotes the net recombination of free carriers per unit volume. The boundary conditions used for the Poisson's equation are:

$$\psi(0) = \phi_{b0} + \chi_0 - \phi_{bL} - \chi_L - V \qquad (6)$$

And

$$\psi(L) = 0 \qquad (7)$$

where Ψ(0) [Ψ(L)] is the vacuum level at x=0 (L), ϕ_{b0} (ϕ_{bL}) the front (back) contact barrier height and χ_0 (χ_L) the electron affinity of the material at x=0 (L).

The typical gap-state distributions used in the calculations consists of U-shaped model, and two Gaussian distribution functions to simulate the dangling bond states. The generation term in the continuity equations has been calculated using a semiempirical model [7] that has been integrated into the modelling program. Both secular interference effects and diffused reflectances and transmittances due to interface roughness are taken into account. The principal parameters used in this study are summarized in table 1.

3. RESULTS AND DISCUSSION

The device used in the present work consists of a HIT structure ITO/n-a-Si:H/i-pm-Si:H/p-c-Si/Al. In these cells, the parameters of each layer are summarized in table 1. The E_{sbb} "Eq. (1)." has been changed to get 0.12 eV < ϕ_{b0} < 0.28 eV. Experimentally, we can change ϕ_{b0} if we interpose a thin Palladium or Chrome film [3,4].

Figure 2 shows recombination variation at the ITO/n-layer interface. We notice a increase of the recombination when we increase the ϕ_{b0} value. This increase of the recombination reduces the flow of electrons to pass from the n-layer to the contact and will affect the variation J(V) characteristics.

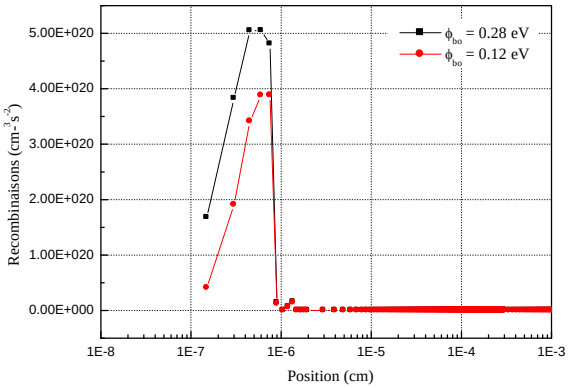

Figure 2: Recombination variation at the ITO/n-layer interface as a function of

Figure 3 shows the open circuit voltage V_{oc} (a), the short circuit current density J_{sc} (c), the fill factor FF and the cell efficiency η (d) as a function of the front contact height barrier ϕ_{b0}. We hardly notice any change on the J(V) characteristics. Indeed, the open circuit voltage V_{oc}, the fill factor FF and the efficiency η remain unchanged.

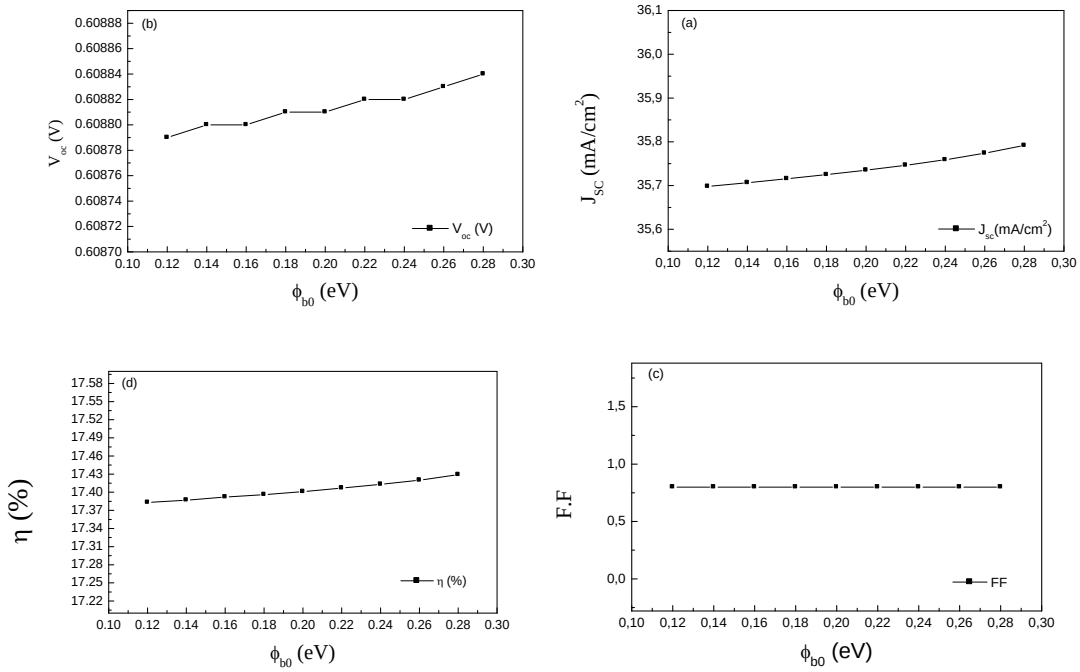

Figure 3: Plot of (a) Short circuit current J_{sc}, (b) V_{oc} Open circuit voltage, (c) Fill Factor FF and, (d) Cell efficiency η as a function of the front contact height barrier ϕ_{b0}.

Figure 4 illustrates the contact ITO/n-a-Si :H at thermodynamic equilibrium for work function of ITO ϕ_{ITO} = 4.30 eV.

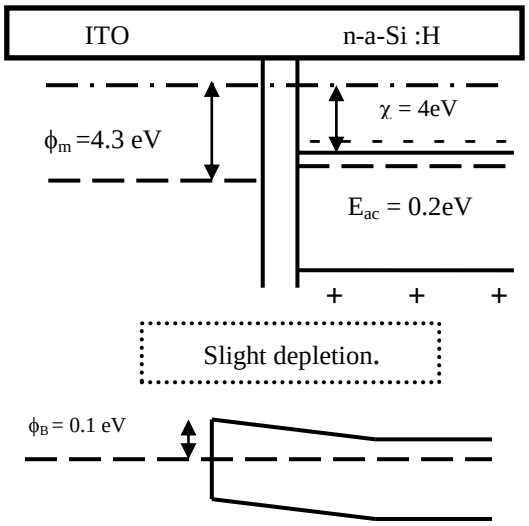

Figure 4: Contact ITO/n-a-Si :H at thermodynamic equilibrium for work function of ITO ϕ_{ITO} = 4.30 eV.

The electron affinity of hydrogenated n-doped amorphous silicon (n-a-Si: H) is between 3.9 and 4 eV and its activation energy is about 0.2 eV, which gives us a work function equal to about 4.20 eV. Knowing that the work function of ITO is higher than the semiconductor ϕ_{ITO} = 4.30 eV, the formation of this contact (ITO/n-a-Si:H) is likely to drive the n-layer (n-a-Si:H) into depletion, causing a drop in open circuit voltage V_{oc}. We consider the potential barrier for such contact between 0.1 and 0.2 eV. An increase of work function of ITO (ϕ_{ITO} = 5 eV Figure 5), led to a sharp depletion of n-layer

which significantly affects the band bending. It grows up, and it only increases the potential barrier, which opposes the diffusion of electrons as shown in Figure 6.

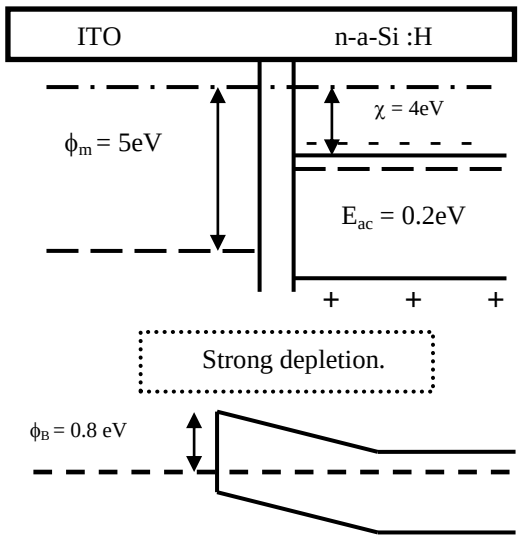

Figure 5: Contact ITO/n-a-Si :H at thermodynamic equilibrium for work function of ITO ϕ_{ITO} = 5 eV.

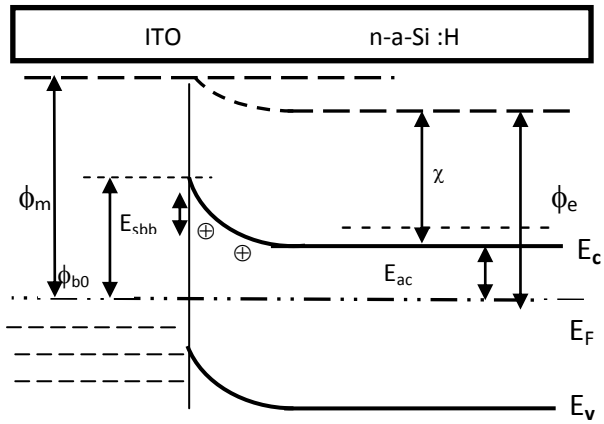

Figure 6 : The schematic band diagram of TCO/n-a-Si:H interface region.

ϕ_m is the work function of TCO, ϕ_e is the work function of n-a-Si:H. ϕ_{b0} is the front contact barrier height, E_{sbb} is the TCO/n-surface band bending, E_{ac} (n) is the activation energy of the n-layer, χ is the electron affinity of the n-a-Si:H.

4. CONCLUSION

In conclusion, we have found that the cell performance doesn't depend on the front contact barrier on ITO/hydrogenated n-doped amorphous silicon heterojunction solar cells. Indeed, we have shown that an increase of the front contact height barrier ϕ_{b0} doesn't lead to a change of the J(V) characteristics. The simplest explanation is that an increase of work function of ITO led to an increase of the recombination that involves a sharp depletion of n-layer and therefore to an increase of the potential barrier.

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