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Influence of the front contact barrier height on the Indium Tin Oxide/hydrogenated p-doped amorphous silicon heterojunction solar cells

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Abstract

The band bending at the transparent conductive oxides/hydrogenated p-doped amorphous silicon (p-a-Si:H) interface is one of the most important factors limiting the performances of HIT (Heterojunctions with Intrinsic Thin layers) solar cells. In order to study this effect, a solar cell (Indium Tin Oxide (ITO)/p-a-Si:H/i-polymorphous Si:H/n-doped crystalline silicon (n-c-Si)) simulation, focused on the front contact barrier height, has been performed. The results show that a reduction of the surface potential barrier at the interface ITO/p-layer leads to an increase of the built-in potential, and hence an increase of open circuit voltage and fill factor. We have also observed that the performance of HIT solar cells remains constant above 12nm thickness of the p-layer.

Keywords: Simulation; HIT solar cells; Potential barrier; Band bending; Current–voltage $J(V)$ characteristics

1. Introduction

The high efficiency of HIT structure (Heterojunctions with Intrinsic Thin layers between the hydrogenated amorphous silicon a-Si:H emitter and crystalline silicon c-Si) for n-type substrates is recently under intensive investigations since they are combining the low cost and low temperature process of a-Si:H deposition coupled with the high efficiency and high stability of c-Si. An important scientific and technological progress on HIT 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/p-doped a-Si:H interface. TCO: Tin Oxide (SnO_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 resistively and high transparency in the visible region. However, many problems are associated with the use of these TCO. One of these problems is the low work function of TCO ($\phi_m \sim 3.70$eV and 4.30eV as an example for SnO_2 and ITO) compared to p-layer ($\phi_s \sim 4.80$eV) [3–5], an electron injection barrier develops at its interface with the p-a-Si:H. This barrier limits the open circuit voltage V_{oc} by a downwards band bending which develops at the TCO/p-a-Si:H interface [3,6–8]. Fig. 1 illustrates the schematic band diagram of interface region.

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

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 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 ϕ_{b0} has to be increased (the downwards band-banding reduced) to increase the efficiency η of the p-i-n solar cells [9]. In order to simulate and study the effect of this barrier in the structure HIT: ITO/p-a-Si:H/i-polymorphous (pm-Si:H)/n-c-Si/Al, we have varied the surface band bending by changing the E_{sbb} in order to reduce E_b between the ITO and p-layer. We chose the pm-Si:H as an intrinsic thin layer because of its excellent electric properties [10].

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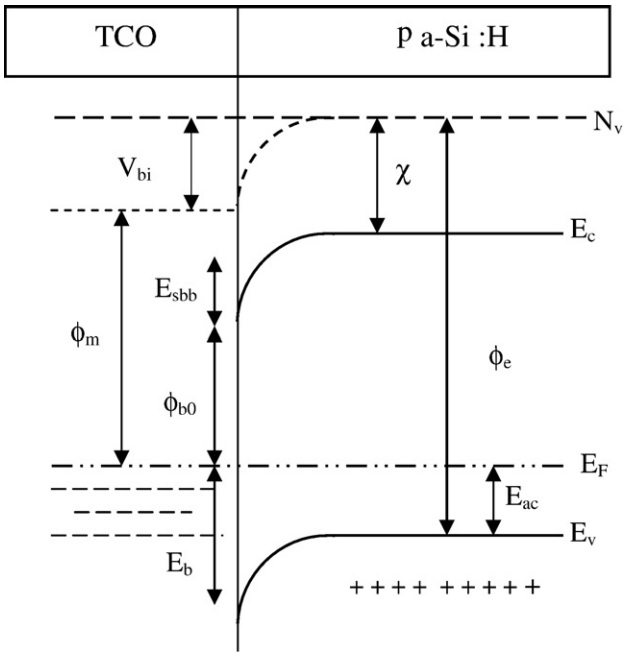

Fig. 1. The schematic band diagram of TCO/p-a-Si:H interface region.

We have used the ASDMP simulation model (Amorphous Semiconductor Device Modeling Program) developed by Professor Parsathi Chatterjee's group [11–13]. 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 cells with data from solar cell performance [14,15].

2. Simulation model

The ASDMP model 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 current–voltage $J(V)$ characteristics and the quantum efficiency.

These equations are:

$$\frac{d}{dx}\left(\varepsilon(x)\frac{d\psi(x)}{dx}\right) = \rho(x). \tag{1}$$

$$0 = \frac{1}{q}\frac{dJ_n(x)}{dx} + G_{\text{opt}}(x) - R_{\text{net}}(x). \tag{2}$$

$$0 = \frac{1}{q}\frac{dJ_p(x)}{dx} + G_{\text{opt}}(x) - R_{\text{net}}(x). \tag{3}$$

In Poisson's equation [Eq. (1)], $\varepsilon(x)$ is the dielectric permittivity of the semiconductor. $\Psi(x)$ is the potential energy of an electron at the vacuum level in electron volts, and $\rho(x)$ is the space charge density in the semiconductor. In the continuity equations [Eqs. (2), (3)], $J_n(x)$ and $J_p(x)$ are the electron and hole current, respectively, and q is the charge of electron. The term $G_{\text{net}}(x)$ represents the net optical generation of free electron-hole pairs per unit volume, while $R_{\text{net}}(x)$ denotes the net recombination of free carriers per unit volume. The expression of free and trapped charges, the recombination term, the boundary conditions and the solution technique in this program, are similar to the AMPS computer program [16–18] developed by Professor Fonash's group. We mentioned bellow the four boundary conditions for the hole- and electron-continuity equations:

$$J_p(0) = q\mu_p p_{\text{NE}}(0)\frac{\partial E_{\text{FN}}}{\partial x}\Big|_{x=0} = -qS_{p0}[p_{\text{NE}}(0) - p_0(0)]. \tag{4}$$

$$J_n(0) = q\mu_n p_{\text{NE}}(0)\frac{\partial E_{\text{Fn}}}{\partial x}\Big|_{x=0} = -qS_{n0}[n_{\text{NE}}(0) - n_0(0)]. \tag{5}$$

$$J_p(L) = q\mu_p p_{\text{NE}}(L)\frac{\partial E_{\text{Fp}}}{\partial x}\Big|_{x=0} = -qS_{pL}[p_{\text{NE}}(L) - p_0(L)]. \tag{6}$$

$$J_n(L) = q\mu_n n_{\text{NE}}(L)\frac{\partial E_{\text{Fn}}}{\partial x}\Big|_{x=0} = -qS_{nL}[n_{\text{NE}}(L) - n_0(L)]. \tag{7}$$

Where q is the electronic charge, μ_p (μ_n) the hole (electron) band microscopic mobilities, and E_{Fp} (E_{Fn}) the quasi-Fermi level for holes (electrons). $J_p(0)$, $J_p(L)$ and $J_n(0)$, $J_n(L)$ represent the hole and electron current densities, respectively, at $x = 0$ and $x = L$, while p(0), p(L) and n(0), n(L) are the hole and electron free carrier densities at $x = 0$ and $x = L$. The subscript ''NE'' represents the respective values at the nonthermodynamic equilibrium steady state, while the subscript ''0'' represents the values at thermodynamic equilibrium. S_{p0}, S_{pL}, S_{n0}, and S_{nL} are the surface recombination speeds of holes at $x = 0$, $x = L$, and of electrons at $x = 0$, $x = L$, respectively. $x = 0$ represents the point where the light enters and where the voltage is applied, the other end of the device ($x = L$) being at ground potential. The boundary conditions used for the Poisson's equation are:

$$\psi(0) = \phi_{b0} + \chi_0 - \phi_{bL} - \chi_L - V \tag{8}$$

And

$$\psi(L) = 0 \tag{9}$$

Where $\Psi(0)$ [$\Psi(L)$] 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). For light through the p-layer, ϕ_{b0} and χ_0 represent the contact barrier height and the electron affinity of the p-a-Si:H layer, while ϕ_{bL} and χ_L are those of n-a-Si:H. V is the applied forward biased potential. The contact barrier heights for a cell with the p-layer in contact with a TCO at $x = 0$ and the n-layer in contact with a metal at $x = L$, are given by:

$$\phi_{b0} = E_\mu(p) - E_{ac}(p) - E_{sbb} \tag{10}$$

And

$$\phi_{bL} = E_{ac}(n) \tag{11}$$